



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 06:46 PM EST

PDB ID : 1VQ9  
Title : The structure of CCA-PHE-CAP-BIO and the antibiotic sparsomycin bound to the large ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.40 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](mailto: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>.

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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 : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

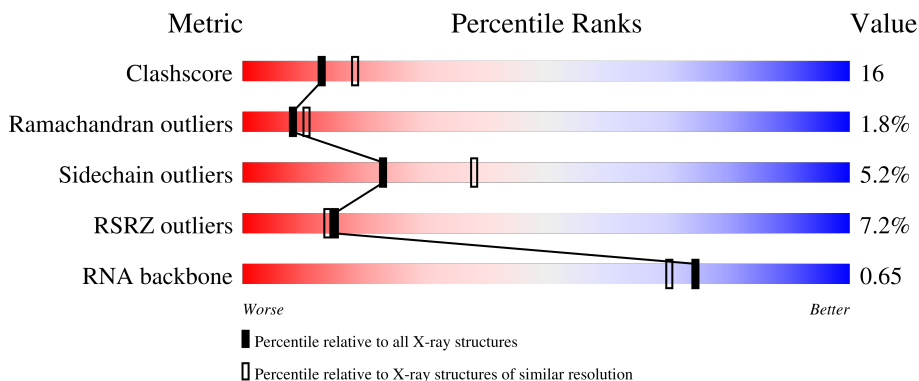
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.



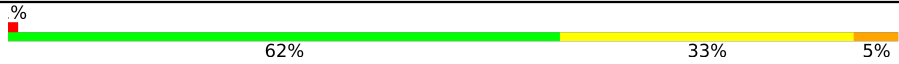
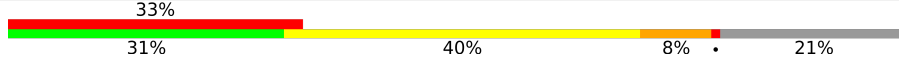
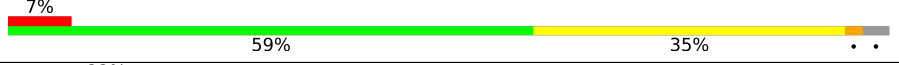
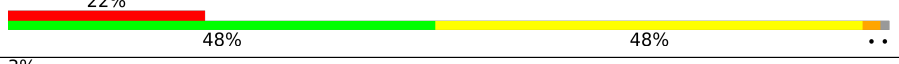
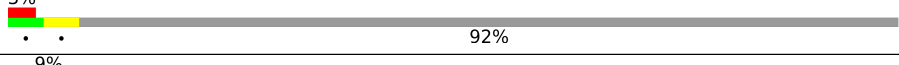
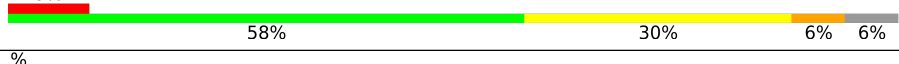
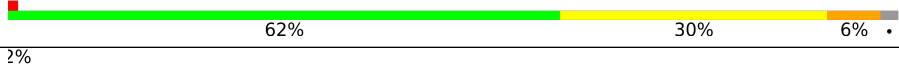

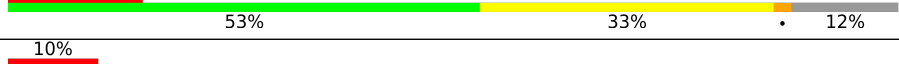


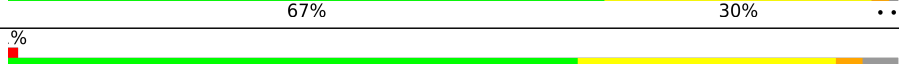
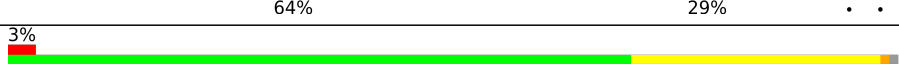
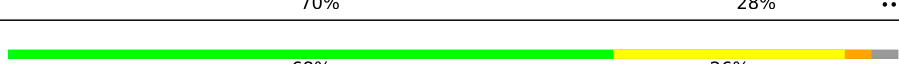



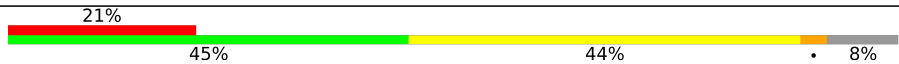


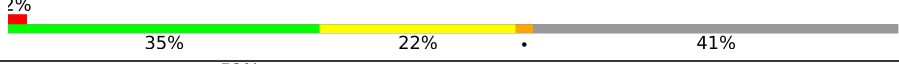
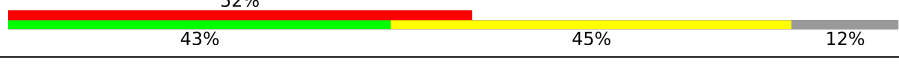
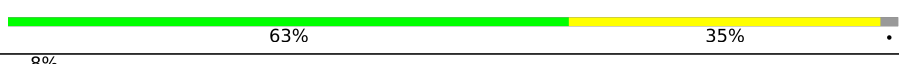


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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  $\geq 3$ , 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	0	2922	 2% 58% 30% 5% 6%
2	9	122	 4% 53% 34% 11%
3	4	5	 80% 20%
4	A	240	 9% 53% 41% 5%
5	B	338	 54% 41% 5%

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Mol	Chain	Length	Quality of chain
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	

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Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8024	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8108	-	-	-	X
35	NA	0	9102	-	-	-	X
35	NA	0	9132	-	-	-	X
35	NA	0	9172	-	-	-	X
35	NA	0	9184	-	-	-	X
37	SR	0	9482	-	-	-	X
37	SR	0	9601	-	-	-	X
37	SR	B	9521	-	-	-	X

## 2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 98979 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2754	59021	26350	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	9	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a RNA chain called 5'-R(\*CP\*CP\*AP\*(PHE)\*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	5	74	40	12	20	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	A	237	1753	1072	352	324	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	B	337	2625	1616	493	511	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	246	1859	1131	344	383	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	D	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	E	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	F	119	890	551	141	197	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	G	29	240	149	39	51	1	0	0	0

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	H	160	1266	785	237	238	6	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	J	142	1120	696	199	222	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	K	132	992	609	187	192	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

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

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501
M	194	ALA	GLY	conflict	GB 55231501

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	W	154	1196	737	209	244	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	X	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	Y	142	1130	686	228	216		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	Z	73	578	346	116	111	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	1	56	431	258	86	83	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	2	46	396	239	89	67	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	3	92	755	458	153	137	7	0	0	0

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	I	70	519	323	81	114	1	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	86	Total	Mg	0	0
			86	86		
33	9	1	Total	Mg	0	0
			1	1		
33	4	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	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	62	Total	Na	0	0
			62	62		
35	9	2	Total	Na	0	0
			2	2		
35	B	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	D	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	J	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	R	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	T	1	Total 1	Na 1	0	0
35	3	1	Total 1	Na 1	0	0

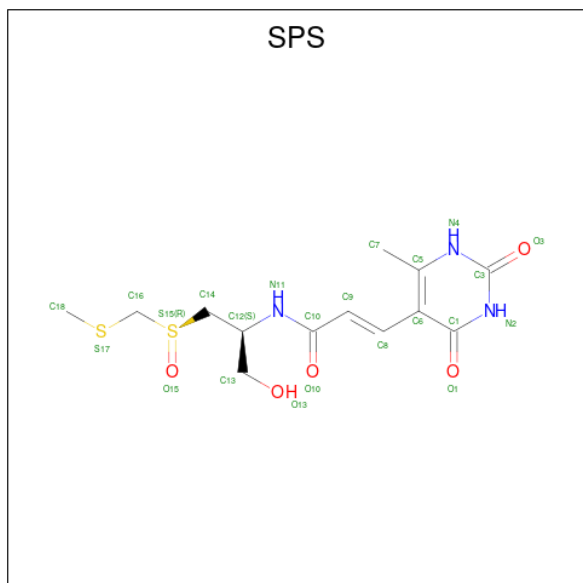
- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	9	Total 9	Cl 9	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	J	3	Total 3	Cl 3	0	0
36	K	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	97	Total Sr 97 97	0	0
37	9	3	Total Sr 3 3	0	0
37	A	4	Total Sr 4 4	0	0
37	B	2	Total Sr 2 2	0	0
37	F	1	Total Sr 1 1	0	0
37	H	1	Total Sr 1 1	0	0
37	L	1	Total Sr 1 1	0	0
37	R	1	Total Sr 1 1	0	0
37	S	1	Total Sr 1 1	0	0
37	1	2	Total Sr 2 2	0	0
37	3	1	Total Sr 1 1	0	0

- Molecule 38 is SPARSOMYCIN (three-letter code: SPS) (formula: C<sub>13</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
38	4	1	23	13	3	5	2	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5630	Total	O	0	0
			5630	5630		
40	9	130	Total	O	0	0
			130	130		
40	4	1	Total	O	0	0
			1	1		
40	A	132	Total	O	0	0
			132	132		
40	B	137	Total	O	0	0
			137	137		
40	C	175	Total	O	0	0
			175	175		
40	D	43	Total	O	0	0
			43	43		
40	E	42	Total	O	0	0
			42	42		
40	F	25	Total	O	0	0
			25	25		
40	G	16	Total	O	0	0
			16	16		
40	H	77	Total	O	0	0
			77	77		
40	J	52	Total	O	0	0
			52	52		

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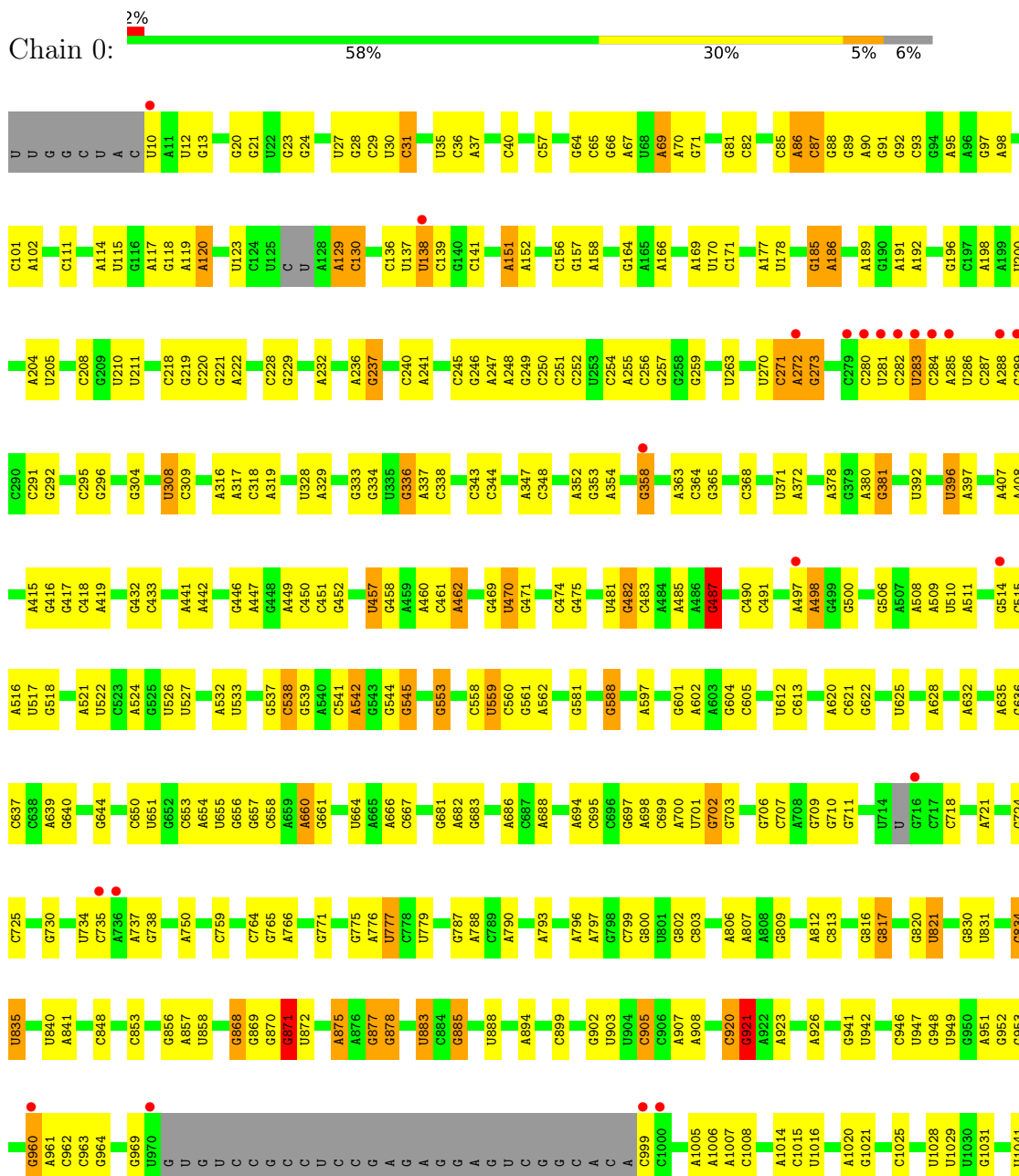
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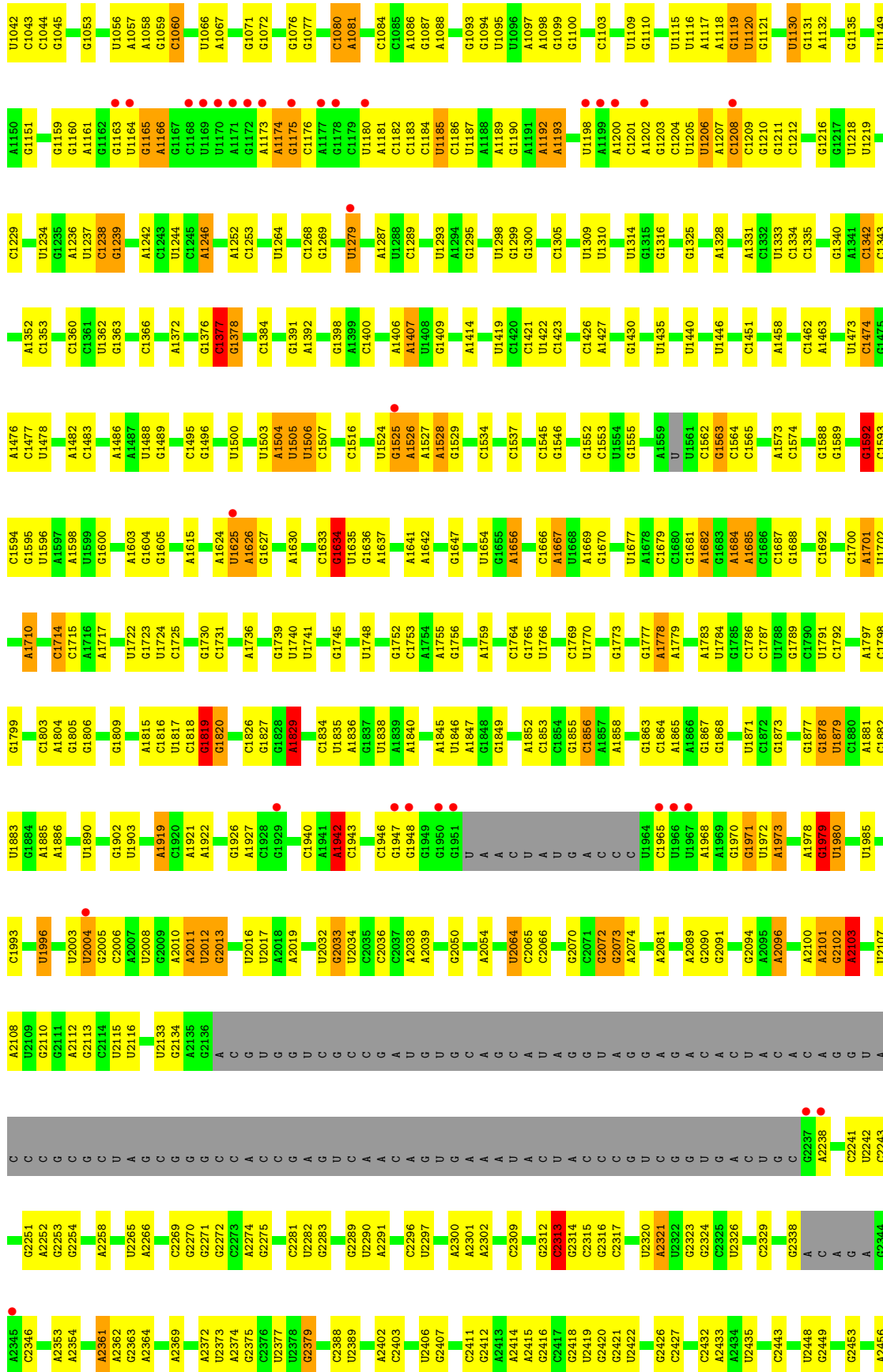
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	K	61	Total O 61 61	0	0
40	L	93	Total O 93 93	0	0
40	M	133	Total O 133 133	0	0
40	N	66	Total O 66 66	0	0
40	O	42	Total O 42 42	0	0
40	P	68	Total O 68 68	0	0
40	Q	53	Total O 53 53	0	0
40	R	93	Total O 93 93	0	0
40	S	35	Total O 35 35	0	0
40	T	40	Total O 40 40	0	0
40	U	28	Total O 28 28	0	0
40	V	13	Total O 13 13	0	0
40	W	70	Total O 70 70	0	0
40	X	23	Total O 23 23	0	0
40	Y	93	Total O 93 93	0	0
40	Z	30	Total O 30 30	0	0
40	1	60	Total O 60 60	0	0
40	2	46	Total O 46 46	0	0
40	3	70	Total O 70 70	0	0
40	I	9	Total O 9 9	0	0

### 3 Residue-property plots i

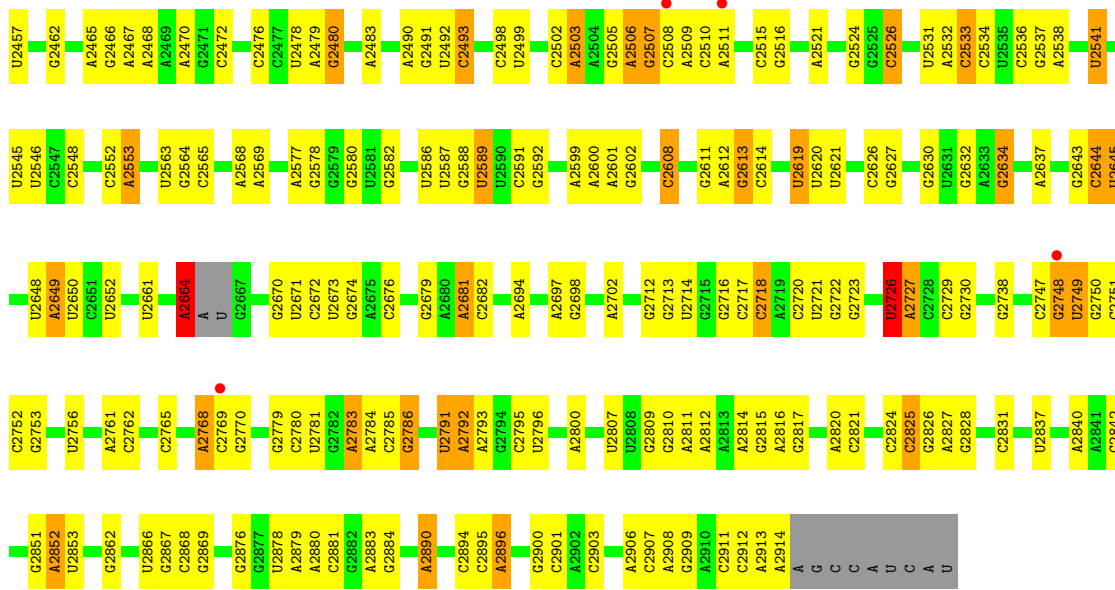
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S ribosomal rna

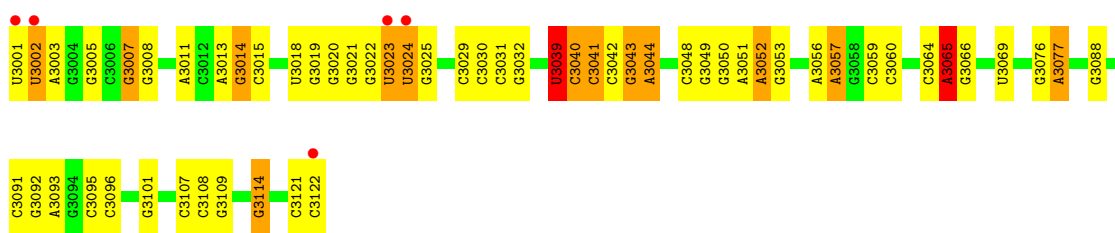




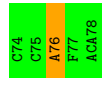
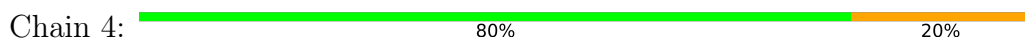




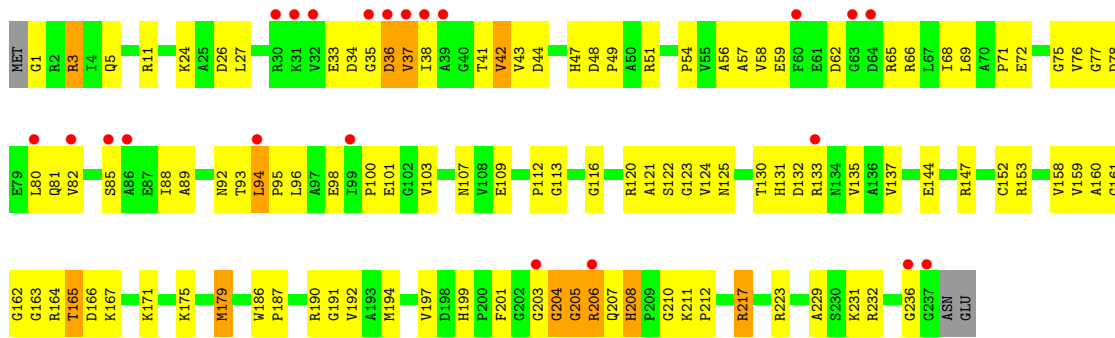
• Molecule 2: 5S ribosomal RNA



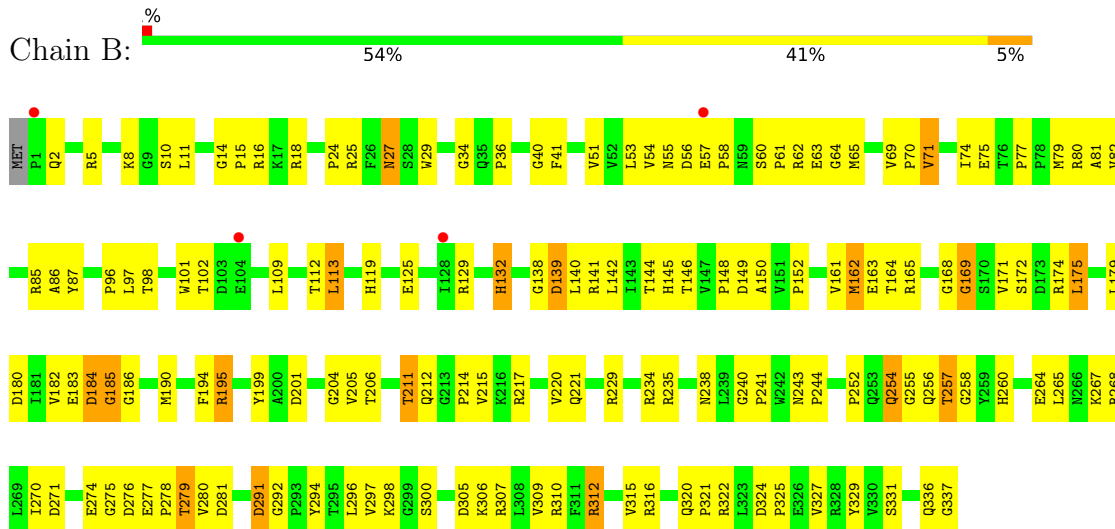
• Molecule 3: 5'-R(\*CP\*CP\*AP\*(PHE)\*(ACA))-3'



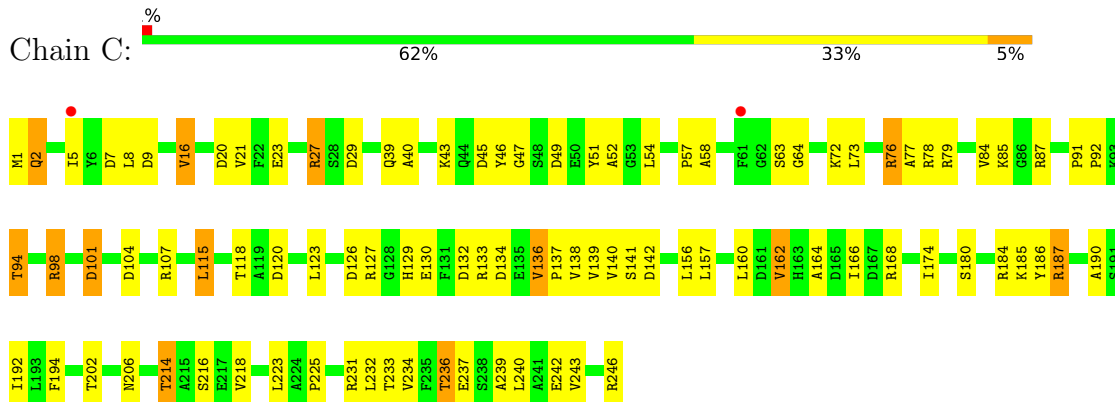
• Molecule 4: 50S ribosomal protein L2P



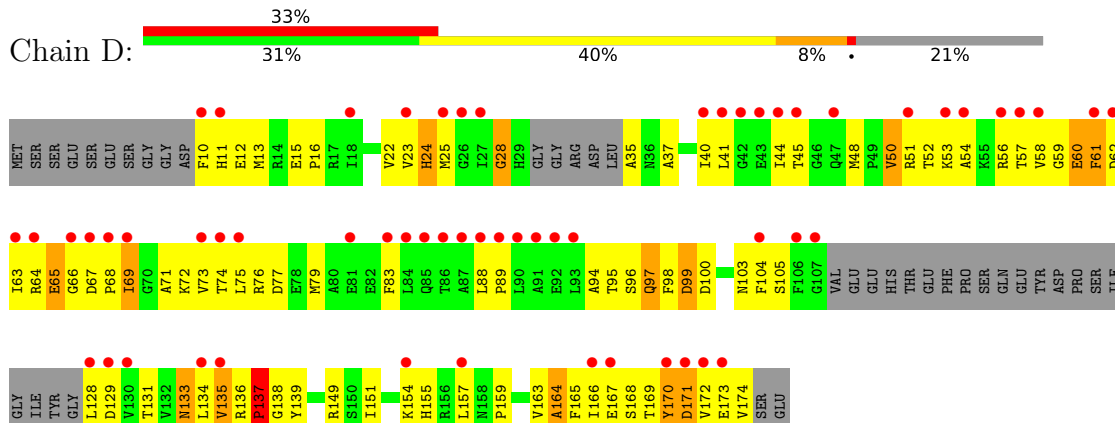
• Molecule 5: 50S ribosomal protein L3P



• Molecule 6: 50S ribosomal protein L4E

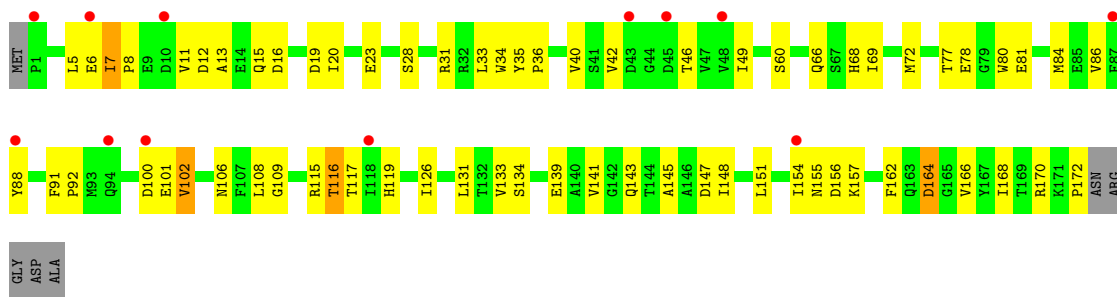


• Molecule 7: 50S ribosomal protein L5P

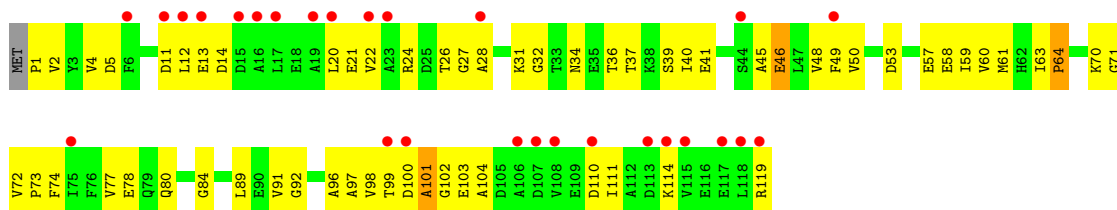


• Molecule 8: 50S ribosomal protein L6P

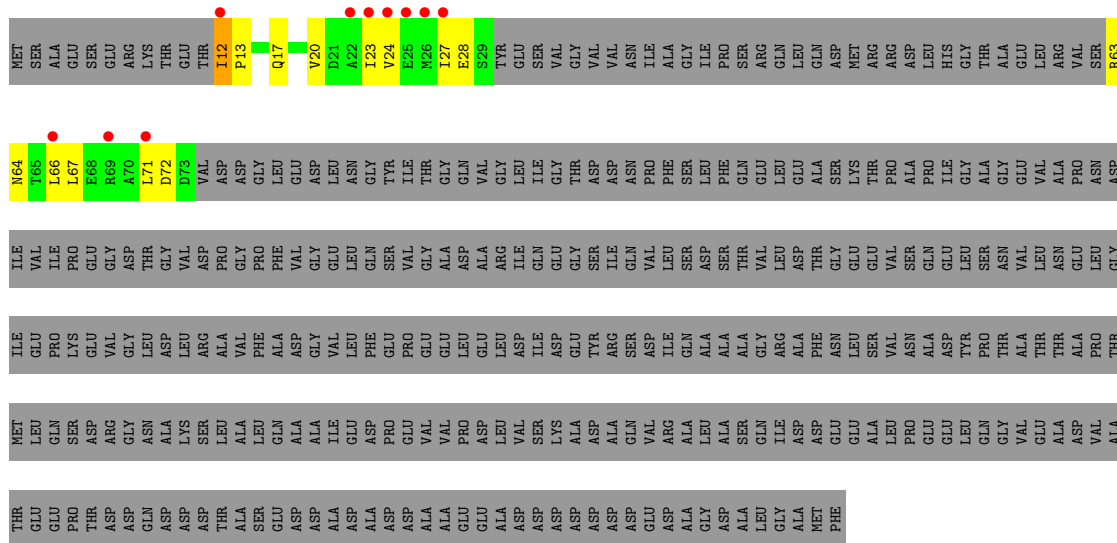




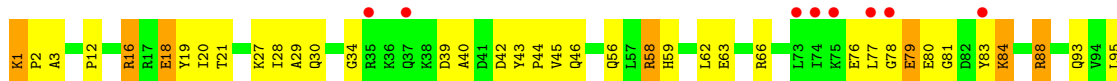
Molecule 9: 50S ribosomal protein L7AE

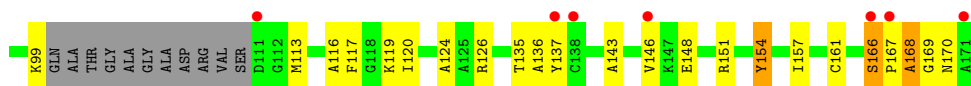


Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

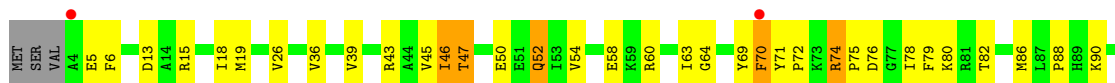


Molecule 11: 50S RIBOSOMAL PROTEIN L10E

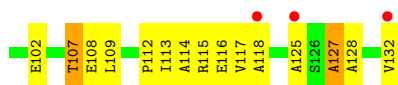




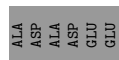
- Molecule 12: 50S ribosomal protein L13P



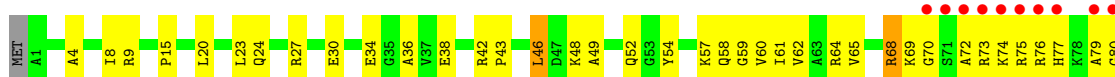
- Molecule 13: 50S ribosomal protein L14P



- Molecule 14: 50S ribosomal protein L15P



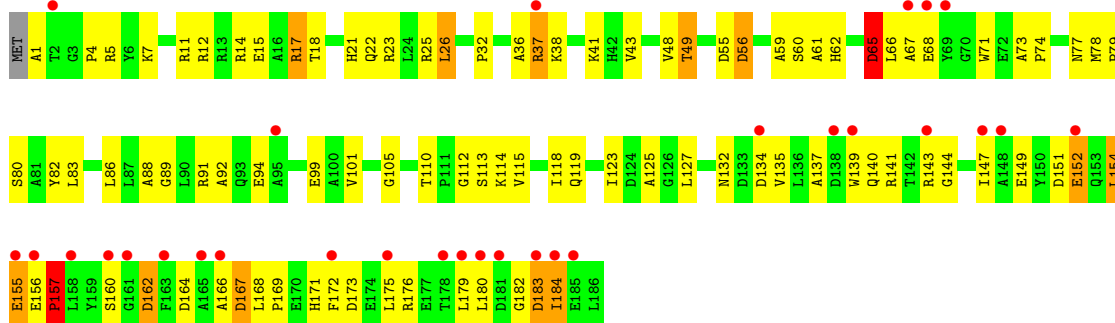
- Molecule 15: 50S Ribosomal Protein L15E



K193  
A194

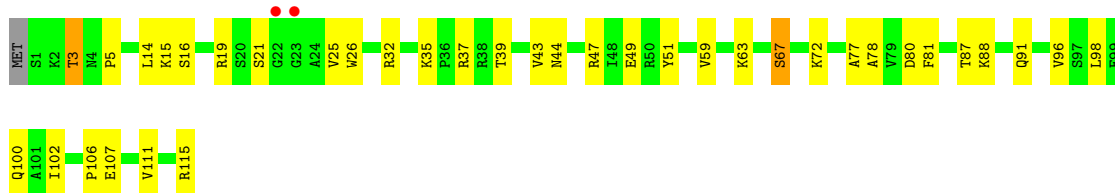
## ● Molecule 16: 50S ribosomal protein L18P

Chain N: 16% 49% 43% 6% ..



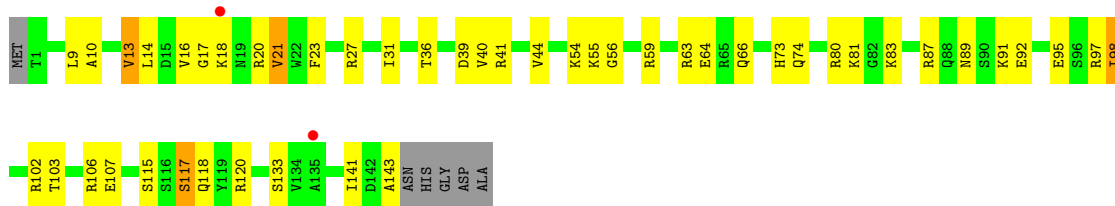
## ● Molecule 17: 50S ribosomal protein L18e

Chain O: 2% 67% 30% ..



## ● Molecule 18: 50S ribosomal protein L19E

Chain P: 1% 64% 29% ..



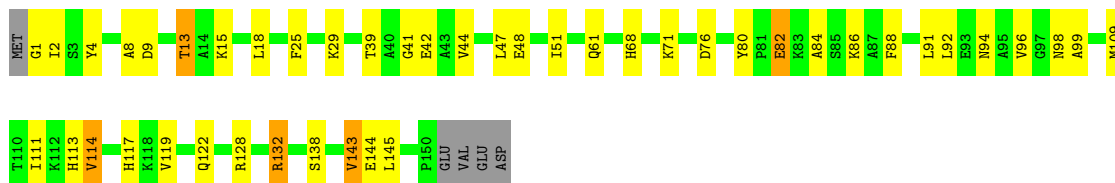
## ● Molecule 19: 50S ribosomal protein L21e

Chain Q: 3% 70% 28% ..

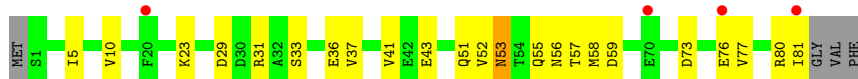


## ● Molecule 20: 50S ribosomal protein L22P

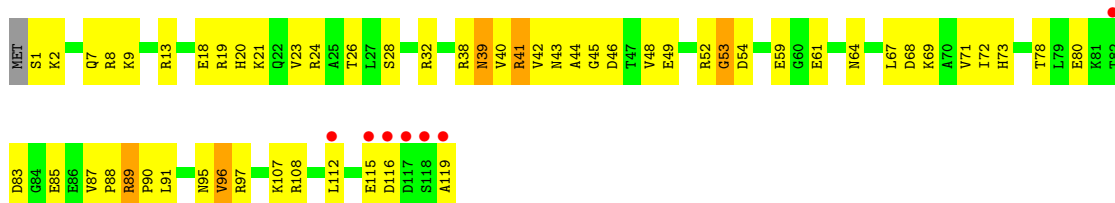
Chain R: 68% 26% ..



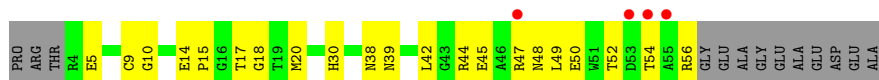
• Molecule 21: 50S ribosomal protein L23P



• Molecule 22: 50S ribosomal protein L24P



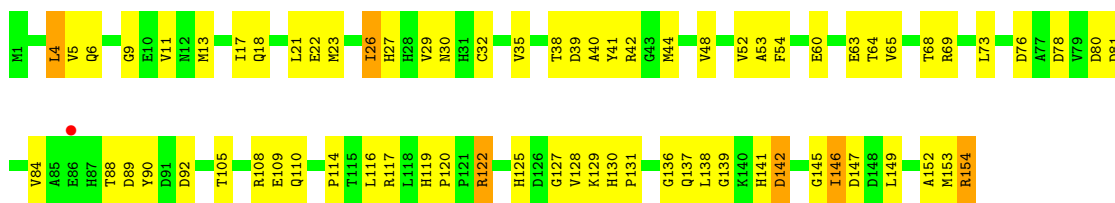
• Molecule 23: 50S ribosomal protein L24E



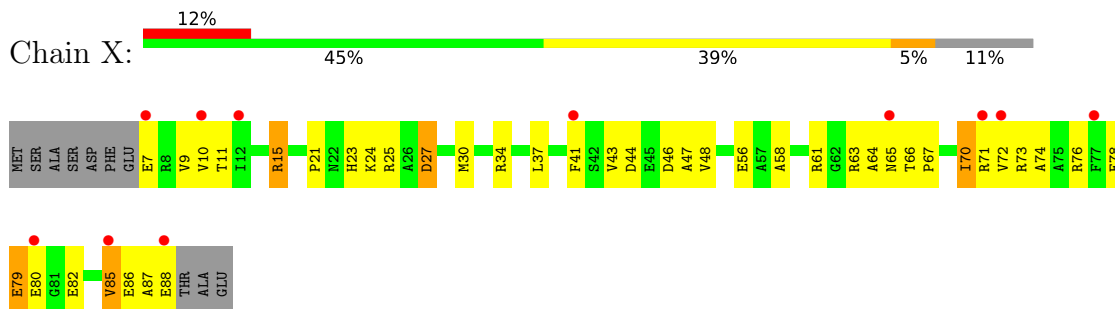
• Molecule 24: 50S ribosomal protein L29P



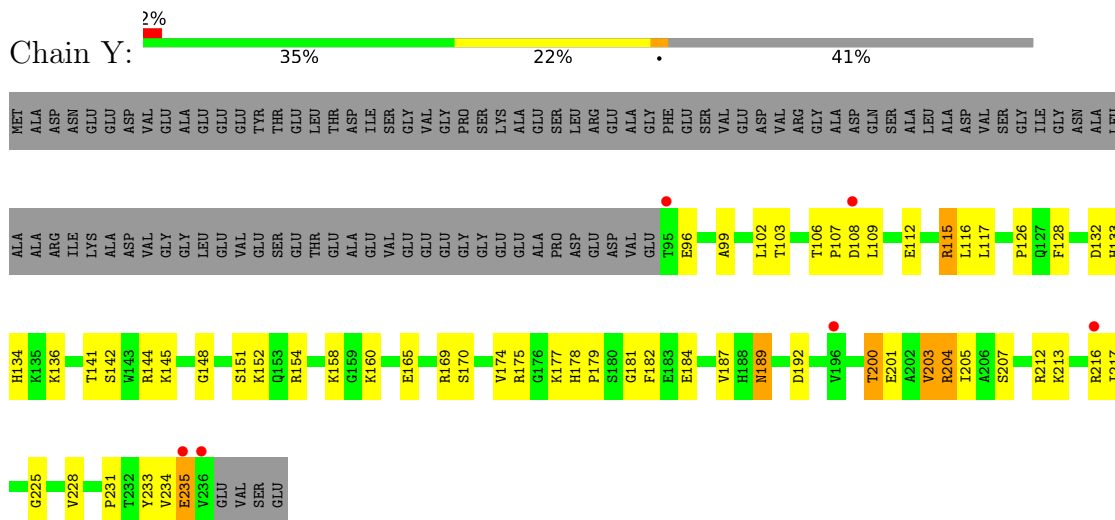
• Molecule 25: 50S ribosomal protein L30P



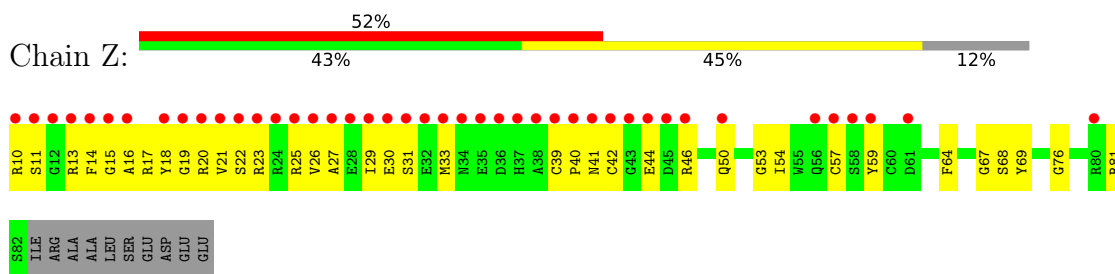
- Molecule 26: 50S ribosomal protein L31e



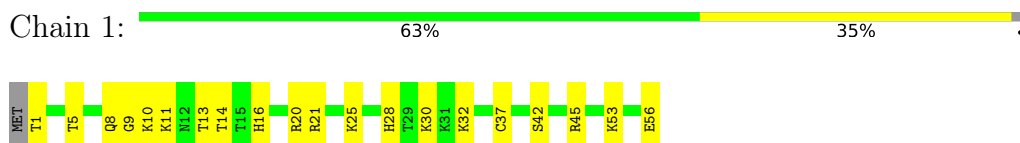
- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae



- Molecule 29: 50S ribosomal protein L37e

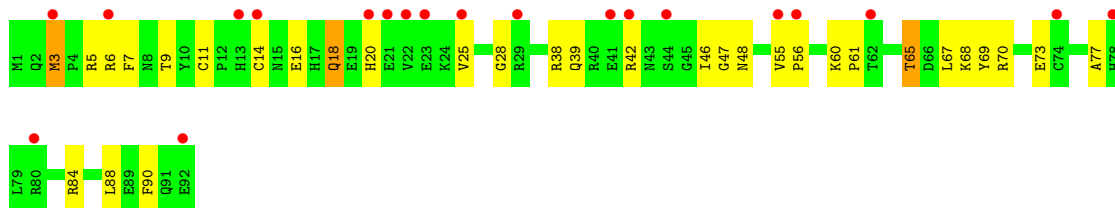


- Molecule 30: 50S ribosomal protein L39e

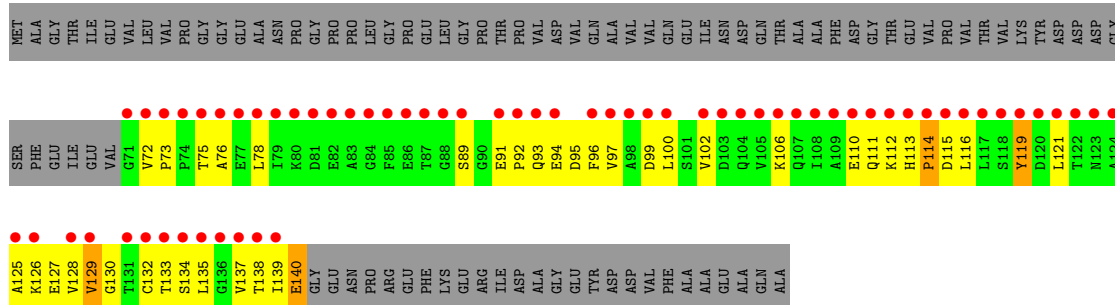
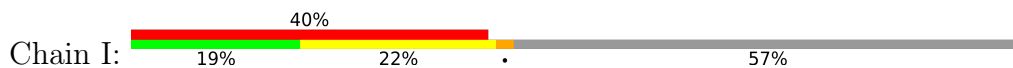




• Molecule 31: 50S ribosomal protein L44E



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.82Å 298.60Å 574.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.68 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.40) 89.6 (49.68-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.59 (at 2.39Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.222 , 0.255 0.220 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtrriage
Anisotropy	0.188	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	98979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SR, CL, PSU, SPS, CD, 1MA, NA, K, OMG, OMU, MG, ACA, UR3

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	0/65959	0.71	23/102870 (0.0%)
2	9	0.39	0/2905	0.73	1/4528 (0.0%)
3	4	0.50	0/76	0.74	0/112
4	A	0.34	0/1786	0.64	0/2408
5	B	0.36	0/2690	0.67	0/3652
6	C	0.39	0/1884	0.66	0/2551
7	D	0.34	0/1111	0.57	0/1498
8	E	0.37	0/1382	0.61	0/1880
9	F	0.36	0/901	0.57	0/1224
10	G	0.33	0/241	0.49	0/324
11	H	0.37	0/1287	0.66	0/1725
12	J	0.38	0/1136	0.64	0/1530
13	K	0.38	0/1001	0.68	0/1347
14	L	0.36	0/1130	0.66	0/1509
15	M	0.38	0/1584	0.61	0/2119
16	N	0.32	0/1474	0.63	0/1999
17	O	0.35	0/874	0.62	0/1181
18	P	0.36	0/1147	0.59	0/1528
19	Q	0.36	0/749	0.68	0/1005
20	R	0.37	0/1172	0.68	0/1578
21	S	0.37	0/648	0.60	0/875
22	T	0.34	0/958	0.63	0/1289
23	U	0.38	0/417	0.56	0/562
24	V	0.31	0/502	0.56	0/675
25	W	0.37	0/1219	0.64	0/1655
26	X	0.38	0/664	0.63	0/895
27	Y	0.39	0/1146	0.68	0/1536
28	Z	0.36	0/589	0.58	0/787
29	1	0.45	0/438	0.68	0/578
30	2	0.38	0/401	0.63	0/529
31	3	0.36	0/771	0.55	0/1024
32	I	0.32	0/526	0.55	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.40	0/98768	0.69	24/147689 (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	1	44
2	9	0	1
All	All	1	45

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.83	131.13	109.50
1	0	871	G	C5'-C4'-O4'	-7.12	100.56	109.10
2	9	3039	U	N1-C1'-C2'	7.04	123.15	114.00
1	0	1979	G	C2'-C3'-O3'	6.99	124.88	113.70
1	0	883	U	N1-C1'-C2'	6.65	122.64	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	460	A	Sidechain
1	0	462	A	Sidechain
1	0	469	G	Sidechain

## 5.2 Too-close contacts [\(i\)](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29809	911	0
2	9	2600	0	1326	55	0
3	4	74	0	42	1	0
4	A	1753	0	1765	133	0
5	B	2625	0	2531	156	0
6	C	1859	0	1816	118	0
7	D	1094	0	1085	94	0
8	E	1357	0	1266	67	0
9	F	890	0	843	62	0
10	G	240	0	231	14	0
11	H	1266	0	1268	62	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	60	0
14	L	1118	0	1076	65	0
15	M	1560	0	1567	91	0
16	N	1445	0	1401	96	0
17	O	865	0	873	46	0
18	P	1136	0	1123	44	0
19	Q	735	0	729	23	0
20	R	1149	0	1122	47	0
21	S	641	0	605	24	0
22	T	950	0	923	73	0
23	U	410	0	364	24	0
24	V	499	0	511	38	0
25	W	1196	0	1137	99	0
26	X	654	0	653	35	0
27	Y	1130	0	1133	67	0
28	Z	578	0	542	42	0
29	1	431	0	426	27	0
30	2	396	0	413	29	0
31	3	755	0	728	43	0
32	I	519	0	500	40	0
33	0	86	0	0	0	0
33	4	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	2	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	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	3	1	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	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	2	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	9	0	0	0	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	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	97	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	4	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	4	23	0	19	3	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	5630	0	0	126	0
40	1	60	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2	46	0	0	1	0
40	3	70	0	0	6	0
40	4	1	0	0	0	0
40	9	130	0	0	5	0
40	A	132	0	0	13	0
40	B	137	0	0	22	0
40	C	175	0	0	20	0
40	D	43	0	0	8	0
40	E	42	0	0	2	0
40	F	25	0	0	4	0
40	G	16	0	0	2	0
40	H	77	0	0	4	0
40	I	9	0	0	0	0
40	J	52	0	0	1	0
40	K	61	0	0	7	1
40	L	93	0	0	11	0
40	M	133	0	0	8	0
40	N	66	0	0	5	0
40	O	42	0	0	5	0
40	P	68	0	0	3	0
40	Q	53	0	0	2	0
40	R	93	0	0	5	0
40	S	35	0	0	2	0
40	T	40	0	0	4	0
40	U	28	0	0	2	0
40	V	13	0	0	1	0
40	W	70	0	0	4	0
40	X	23	0	0	3	0
40	Y	93	0	0	9	0
40	Z	30	0	0	5	0
All	All	98979	0	59956	2476	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 16.

The worst 5 of 2476 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)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.29	1.15
1:O:1160:G:H5'	1:O:1161:A:H5'	1.27	1.13
15:M:68:ARG:HH21	15:M:73:ARG:HD3	1.12	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:236:THR:HG22	6:C:239:ALA:H	1.06	1.12
9:F:91:VAL:HG12	9:F:92:GLY:H	1.12	1.11

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)
40:K:6344:HOH:O	40:K:6344:HOH:O[3_655]	2.05	0.15

## 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	A	235/240 (98%)	208 (88%)	20 (8%)	7 (3%)	<b>4</b> <b>3</b>
5	B	335/338 (99%)	296 (88%)	32 (10%)	7 (2%)	<b>7</b> <b>8</b>
6	C	244/246 (99%)	221 (91%)	22 (9%)	1 (0%)	34 48
7	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	<b>1</b> <b>0</b>
8	E	170/178 (96%)	163 (96%)	7 (4%)	0	<b>100</b> <b>100</b>
9	F	117/120 (98%)	102 (87%)	12 (10%)	3 (3%)	<b>5</b> <b>5</b>
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	<b>100</b> <b>100</b>
11	H	156/171 (91%)	136 (87%)	15 (10%)	5 (3%)	<b>4</b> <b>3</b>
12	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	<b>11</b> <b>15</b>
13	K	130/132 (98%)	118 (91%)	11 (8%)	1 (1%)	19 29
14	L	141/165 (86%)	115 (82%)	25 (18%)	1 (1%)	22 32
15	M	192/195 (98%)	179 (93%)	11 (6%)	2 (1%)	15 23
16	N	184/187 (98%)	158 (86%)	17 (9%)	9 (5%)	<b>2</b> <b>1</b>
17	O	113/116 (97%)	105 (93%)	8 (7%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	P	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
19	Q	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	20
20	R	148/155 (96%)	137 (93%)	10 (7%)	1 (1%)	22	32
21	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
22	T	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	5	5
23	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
24	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	9	13
25	W	152/154 (99%)	145 (95%)	7 (5%)	0	100	100
26	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	12	17
27	Y	140/241 (58%)	135 (96%)	5 (4%)	0	100	100
28	Z	71/83 (86%)	58 (82%)	9 (13%)	4 (6%)	2	1
29	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
30	2	42/50 (84%)	39 (93%)	2 (5%)	1 (2%)	6	6
31	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
32	I	68/162 (42%)	52 (76%)	12 (18%)	4 (6%)	1	0
All	All	3705/4431 (84%)	3338 (90%)	302 (8%)	65 (2%)	8	10

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	36	ASP
4	A	37	VAL
5	B	139	ASP
5	B	169	GLY
7	D	164	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	169 (94%)	10 (6%)	21	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	282/283 (100%)	266 (94%)	16 (6%)	20	33
6	C	193/193 (100%)	176 (91%)	17 (9%)	10	15
7	D	117/148 (79%)	108 (92%)	9 (8%)	13	20
8	E	152/156 (97%)	144 (95%)	8 (5%)	22	37
9	F	93/94 (99%)	92 (99%)	1 (1%)	73	87
10	G	27/283 (10%)	25 (93%)	2 (7%)	13	22
11	H	132/138 (96%)	126 (96%)	6 (4%)	27	44
12	J	118/121 (98%)	106 (90%)	12 (10%)	7	10
13	K	106/106 (100%)	99 (93%)	7 (7%)	16	26
14	L	113/127 (89%)	110 (97%)	3 (3%)	44	65
15	M	158/159 (99%)	153 (97%)	5 (3%)	39	59
16	N	149/150 (99%)	138 (93%)	11 (7%)	13	22
17	O	93/94 (99%)	89 (96%)	4 (4%)	29	46
18	P	113/117 (97%)	109 (96%)	4 (4%)	36	55
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	51
20	R	117/122 (96%)	113 (97%)	4 (3%)	37	56
21	S	71/74 (96%)	70 (99%)	1 (1%)	67	82
22	T	105/106 (99%)	101 (96%)	4 (4%)	33	51
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	48 (94%)	3 (6%)	19	32
25	W	130/130 (100%)	122 (94%)	8 (6%)	18	29
26	X	66/74 (89%)	59 (89%)	7 (11%)	6	9
27	Y	120/196 (61%)	111 (92%)	9 (8%)	13	21
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	40 (95%)	2 (5%)	25	41
31	3	79/79 (100%)	76 (96%)	3 (4%)	33	51
32	I	58/130 (45%)	56 (97%)	2 (3%)	37	56
All	All	3093/3612 (86%)	2932 (95%)	161 (5%)	23	38

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Q	16	ASN
26	X	82	GLU
20	R	82	GLU
25	W	4	LEU
27	Y	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
20	R	113	HIS
25	W	119	HIS
21	S	21	GLN
23	U	39	ASN
27	Y	133	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	249 (9%)	33 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
3	4	2/5 (40%)	1 (50%)	0
All	All	2868/3049 (94%)	268 (9%)	34 (1%)

5 of 268 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 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2718	C
1	0	2726	U
1	0	2852	A
1	0	1237	U
1	0	1165	G

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

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	UR3	0	2619	1	19,22,23	0.48	0	26,32,35	0.63	1 (3%)
1	PSU	0	2621	1	18,21,22	1.52	2 (11%)	22,30,33	1.27	3 (13%)
1	OMU	0	2587	1	19,22,23	0.20	0	26,31,34	0.42	0
1	OMG	0	2588	1	18,26,27	1.03	2 (11%)	19,38,41	0.73	1 (5%)
1	1MA	0	628	35,1	16,25,26	1.47	2 (12%)	18,37,40	1.18	3 (16%)
3	ACA	4	78	3	3,3,8	0.52	0	2,2,8	0.72	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
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	1MA	0	628	35,1	-	0/3/25/26	0/3/3/3
3	ACA	4	78	3	-	0/0/1/6	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.94	1.43	1.36
1	0	628	1MA	C2-N3	4.27	1.34	1.29
1	0	2621	PSU	C6-C5	3.19	1.39	1.35
1	0	2588	OMG	C5-C6	-2.61	1.42	1.47
1	0	628	1MA	C6-N6	2.60	1.34	1.27

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.32	120.52	118.20
1	0	2621	PSU	C6-N1-C2	-3.00	119.61	122.68
1	0	628	1MA	N1-C2-N3	2.72	129.19	126.02
1	0	628	1MA	C5-C6-N1	2.64	117.84	113.90
1	0	2621	PSU	O2-C2-N1	2.54	125.59	122.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2619	UR3	1	0
1	0	2587	OMU	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 313 ligands modelled in this entry, 312 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	SPS	4	9701	33	20,23,23	1.61	4 (20%)	18,30,30	2.78	4 (22%)

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	SPS	4	9701	33	-	5/15/18/18	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	9701	SPS	C6-C1	3.67	1.53	1.43
38	4	9701	SPS	C5-N4	3.11	1.39	1.34
38	4	9701	SPS	C9-C10	-3.01	1.41	1.48
38	4	9701	SPS	C1-N2	2.61	1.37	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	9701	SPS	C6-C1-N2	-8.17	118.70	124.40
38	4	9701	SPS	C3-N2-C1	7.16	121.19	115.14
38	4	9701	SPS	C6-C5-N4	-2.37	119.42	122.12
38	4	9701	SPS	O15-S15-C16	2.10	108.97	106.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	4	9701	SPS	C5-C6-C8-C9
38	4	9701	SPS	N11-C12-C13-O13
38	4	9701	SPS	C14-C12-C13-O13
38	4	9701	SPS	C12-C14-S15-O15
38	4	9701	SPS	C12-C14-S15-C16

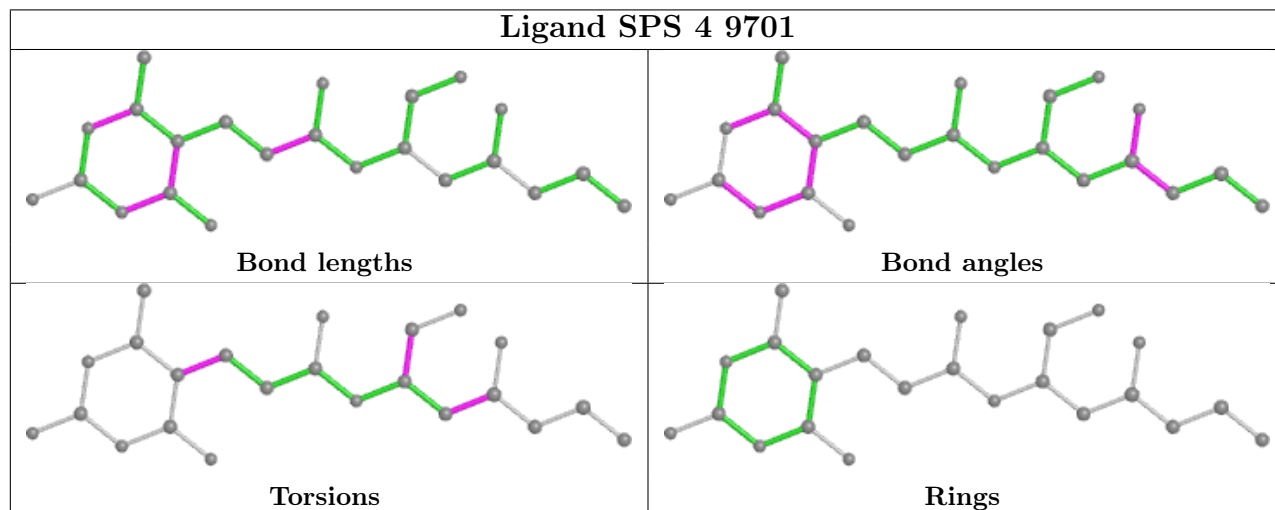
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	4	9701	SPS	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	76:A	O3'	77:PHE	C	1.60

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.61	58 (2%) 63 61	19, 43, 80, 130	0
2	9	122/122 (100%)	-0.36	5 (4%) 37 36	35, 59, 79, 129	0
3	4	4/5 (80%)	0.22	0 100 100	44, 46, 51, 57	0
4	A	237/240 (98%)	0.51	22 (9%) 8 8	28, 51, 79, 92	0
5	B	337/338 (99%)	0.03	4 (1%) 79 77	25, 46, 66, 77	0
6	C	246/246 (100%)	-0.06	2 (0%) 86 84	24, 43, 61, 72	0
7	D	140/177 (79%)	1.90	59 (42%) 0 0	53, 76, 103, 111	0
8	E	172/178 (96%)	0.43	12 (6%) 16 15	37, 55, 69, 73	0
9	F	119/120 (99%)	1.04	27 (22%) 0 0	45, 64, 88, 91	0
10	G	29/348 (8%)	2.24	10 (34%) 0 0	60, 77, 82, 85	0
11	H	160/171 (93%)	0.43	15 (9%) 8 7	39, 54, 80, 84	0
12	J	142/145 (97%)	-0.08	2 (1%) 75 73	32, 43, 59, 75	0
13	K	132/132 (100%)	-0.18	3 (2%) 60 58	30, 42, 59, 67	0
14	L	145/165 (87%)	0.70	25 (17%) 1 1	26, 60, 92, 101	0
15	M	194/195 (99%)	0.61	19 (9%) 7 7	31, 42, 80, 85	0
16	N	186/187 (99%)	0.86	30 (16%) 1 1	43, 58, 93, 98	0
17	O	115/116 (99%)	-0.09	2 (1%) 70 68	36, 49, 61, 67	0
18	P	143/149 (95%)	0.08	2 (1%) 75 73	35, 47, 58, 66	0
19	Q	95/96 (98%)	0.11	3 (3%) 47 46	39, 46, 58, 65	0
20	R	150/155 (96%)	-0.16	0 100 100	27, 39, 56, 67	0
21	S	81/85 (95%)	0.28	4 (4%) 29 28	39, 52, 69, 84	0
22	T	119/120 (99%)	0.42	7 (5%) 22 21	35, 50, 72, 96	0
23	U	53/66 (80%)	0.43	4 (7%) 14 13	39, 50, 66, 72	0
24	V	65/71 (91%)	1.51	15 (23%) 0 0	47, 65, 94, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	-0.10	1 (0%) 89 88	31, 44, 58, 68	0
26	X	82/92 (89%)	0.56	11 (13%) 3 2	37, 49, 69, 85	0
27	Y	142/241 (58%)	0.17	6 (4%) 36 35	24, 41, 57, 76	0
28	Z	73/83 (87%)	3.82	43 (58%) 0 0	63, 85, 94, 98	0
29	1	56/57 (98%)	-0.35	0 100 100	25, 31, 38, 47	0
30	2	46/50 (92%)	0.44	4 (8%) 10 9	32, 51, 65, 70	0
31	3	92/92 (100%)	1.37	20 (21%) 0 0	48, 65, 72, 81	0
32	I	70/162 (43%)	5.16	64 (91%) 0 0	92, 106, 120, 121	0
All	All	6650/7480 (88%)	0.05	479 (7%) 15 14	19, 47, 85, 130	0

The worst 5 of 479 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	16.4
24	V	1	THR	13.7
28	Z	11	SER	13.1
28	Z	22	SER	12.7
32	I	133	THR	12.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ACA	4	78	4/9	0.88	0.22	52,52,52,52	0
1	OMG	0	2588	24/25	0.97	0.12	31,32,34,36	0
1	1MA	0	628	23/24	0.98	0.14	27,30,32,32	0
1	UR3	0	2619	21/22	0.98	0.14	30,33,37,40	0
1	PSU	0	2621	20/21	0.98	0.14	32,35,39,40	0
1	OMU	0	2587	21/22	0.98	0.12	31,34,36,38	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
37	SR	B	9521	1/1	0.32	0.53	196,196,196,196	0
35	NA	0	9122	1/1	0.33	0.35	75,75,75,75	0
35	NA	0	9184	1/1	0.40	1.39	87,87,87,87	0
35	NA	0	9172	1/1	0.43	0.71	76,76,76,76	0
37	SR	0	9484	1/1	0.45	0.14	148,148,148,148	0
33	MG	0	8102	1/1	0.47	0.20	94,94,94,94	0
33	MG	0	8047	1/1	0.47	0.83	92,92,92,92	0
37	SR	0	9501	1/1	0.57	0.25	193,193,193,193	0
35	NA	S	9112	1/1	0.58	0.21	71,71,71,71	0
33	MG	0	8108	1/1	0.58	0.41	88,88,88,88	0
37	SR	0	9590	1/1	0.59	0.12	131,131,131,131	0
37	SR	A	9537	1/1	0.60	0.11	159,159,159,159	0
33	MG	B	8055	1/1	0.60	0.21	85,85,85,85	0
33	MG	0	8050	1/1	0.62	0.26	91,91,91,91	0
37	SR	0	9601	1/1	0.62	0.93	196,196,196,196	0
33	MG	0	8113	1/1	0.64	0.21	78,78,78,78	0
37	SR	9	9588	1/1	0.68	0.14	132,132,132,132	0
35	NA	0	9129	1/1	0.69	0.24	74,74,74,74	0
37	SR	0	9547	1/1	0.71	0.30	175,175,175,175	0
35	NA	0	9132	1/1	0.71	0.55	77,77,77,77	0
34	K	0	9002	1/1	0.75	0.28	91,91,91,91	0
37	SR	0	9482	1/1	0.75	0.47	175,175,175,175	0
37	SR	0	9468	1/1	0.76	0.09	113,113,113,113	0
33	MG	0	8024	1/1	0.77	0.65	87,87,87,87	0
35	NA	0	9102	1/1	0.77	0.45	68,68,68,68	0
35	NA	0	9171	1/1	0.77	0.15	67,67,67,67	0
33	MG	0	8101	1/1	0.77	0.16	68,68,68,68	0
33	MG	0	8045	1/1	0.80	0.24	73,73,73,73	0
33	MG	0	8075	1/1	0.80	0.11	49,49,49,49	0
33	MG	0	8040	1/1	0.81	0.31	73,73,73,73	0
33	MG	0	8090	1/1	0.81	0.32	67,67,67,67	0
35	NA	0	9174	1/1	0.81	0.61	67,67,67,67	0
37	SR	0	9490	1/1	0.82	0.11	129,129,129,129	0
33	MG	0	8093	1/1	0.82	0.11	45,45,45,45	0
35	NA	0	9185	1/1	0.83	0.64	53,53,53,53	0
39	CD	O	9205	1/1	0.83	0.41	196,196,196,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8115	1/1	0.84	0.12	58,58,58,58	0
35	NA	3	9169	1/1	0.84	0.34	84,84,84,84	0
35	NA	0	9177	1/1	0.84	0.54	76,76,76,76	0
35	NA	0	9181	1/1	0.84	0.18	58,58,58,58	0
33	MG	0	8057	1/1	0.84	0.24	64,64,64,64	0
33	MG	0	8104	1/1	0.84	0.21	58,58,58,58	0
35	NA	B	9161	1/1	0.84	0.52	73,73,73,73	0
33	MG	0	8103	1/1	0.85	0.18	53,53,53,53	0
35	NA	0	9164	1/1	0.85	0.51	56,56,56,56	0
33	MG	0	8083	1/1	0.85	0.18	51,51,51,51	0
33	MG	0	8097	1/1	0.85	0.26	65,65,65,65	0
33	MG	0	8088	1/1	0.85	0.10	42,42,42,42	0
33	MG	0	8060	1/1	0.85	0.21	88,88,88,88	0
33	MG	0	8052	1/1	0.86	0.27	75,75,75,75	0
33	MG	0	8107	1/1	0.86	0.19	61,61,61,61	0
35	NA	0	9182	1/1	0.86	0.19	68,68,68,68	0
33	MG	0	8094	1/1	0.86	0.26	65,65,65,65	0
35	NA	0	9125	1/1	0.87	0.66	93,93,93,93	0
35	NA	9	9152	1/1	0.87	0.29	59,59,59,59	0
37	SR	0	9505	1/1	0.87	0.10	117,117,117,117	0
35	NA	0	9126	1/1	0.87	0.11	49,49,49,49	0
37	SR	0	9581	1/1	0.87	0.04	105,105,105,105	0
35	NA	0	9101	1/1	0.87	0.15	41,41,41,41	0
35	NA	0	9179	1/1	0.87	0.79	94,94,94,94	0
37	SR	0	9425	1/1	0.87	0.14	151,151,151,151	0
33	MG	0	8014	1/1	0.87	0.36	74,74,74,74	0
35	NA	0	9107	1/1	0.87	0.34	52,52,52,52	0
33	MG	0	8099	1/1	0.87	0.29	77,77,77,77	0
35	NA	0	9150	1/1	0.88	0.22	44,44,44,44	0
35	NA	0	9154	1/1	0.88	0.30	54,54,54,54	0
35	NA	0	9175	1/1	0.88	0.18	42,42,42,42	0
35	NA	0	9155	1/1	0.88	0.25	65,65,65,65	0
35	NA	0	9159	1/1	0.88	0.46	56,56,56,56	0
33	MG	0	8092	1/1	0.88	0.52	68,68,68,68	0
35	NA	0	9127	1/1	0.88	0.35	75,75,75,75	0
33	MG	0	8076	1/1	0.89	0.20	57,57,57,57	0
35	NA	0	9163	1/1	0.89	0.19	72,72,72,72	0
35	NA	9	9183	1/1	0.89	0.18	84,84,84,84	0
37	SR	9	9503	1/1	0.89	0.06	105,105,105,105	0
35	NA	0	9139	1/1	0.89	0.15	61,61,61,61	0
33	MG	0	8065	1/1	0.89	0.31	92,92,92,92	0
33	MG	0	8046	1/1	0.89	0.16	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8089	1/1	0.89	0.20	54,54,54,54	0
37	SR	0	9570	1/1	0.90	0.11	117,117,117,117	0
33	MG	0	8054	1/1	0.90	0.11	61,61,61,61	0
35	NA	0	9149	1/1	0.90	0.10	46,46,46,46	0
35	NA	0	9110	1/1	0.90	0.22	39,39,39,39	0
33	MG	0	8041	1/1	0.90	0.12	52,52,52,52	0
37	SR	0	9465	1/1	0.90	0.12	105,105,105,105	0
37	SR	0	9506	1/1	0.90	0.05	108,108,108,108	0
37	SR	0	9508	1/1	0.90	0.12	87,87,87,87	0
33	MG	0	8022	1/1	0.90	0.51	67,67,67,67	0
35	NA	0	9167	1/1	0.91	0.14	59,59,59,59	0
35	NA	0	9168	1/1	0.91	0.21	74,74,74,74	0
33	MG	0	8051	1/1	0.91	0.21	24,24,24,24	0
33	MG	0	8085	1/1	0.91	0.35	69,69,69,69	0
35	NA	0	9173	1/1	0.91	0.19	57,57,57,57	0
35	NA	0	9157	1/1	0.91	0.18	35,35,35,35	0
35	NA	0	9141	1/1	0.91	0.09	64,64,64,64	0
35	NA	J	9146	1/1	0.91	0.12	58,58,58,58	0
35	NA	0	9113	1/1	0.91	0.17	67,67,67,67	0
33	MG	0	8112	1/1	0.91	0.08	44,44,44,44	0
37	SR	0	9539	1/1	0.92	0.35	173,173,173,173	0
33	MG	0	8098	1/1	0.92	0.09	40,40,40,40	0
35	NA	0	9111	1/1	0.92	0.11	46,46,46,46	0
33	MG	0	8068	1/1	0.92	0.10	36,36,36,36	0
37	SR	0	9585	1/1	0.92	0.11	91,91,91,91	0
35	NA	0	9114	1/1	0.92	0.21	56,56,56,56	0
35	NA	0	9134	1/1	0.92	0.06	38,38,38,38	0
33	MG	0	8061	1/1	0.92	0.11	78,78,78,78	0
35	NA	0	9140	1/1	0.92	0.41	65,65,65,65	0
35	NA	0	9124	1/1	0.92	0.21	52,52,52,52	0
34	K	0	9001	1/1	0.92	0.32	101,101,101,101	0
37	SR	0	9532	1/1	0.92	0.09	114,114,114,114	0
39	CD	Z	9203	1/1	0.92	0.10	155,155,155,155	0
37	SR	0	9517	1/1	0.93	0.07	94,94,94,94	0
37	SR	0	9529	1/1	0.93	0.16	123,123,123,123	0
37	SR	0	9530	1/1	0.93	0.16	107,107,107,107	0
35	NA	0	9158	1/1	0.93	0.33	46,46,46,46	0
36	CL	3	9304	1/1	0.93	0.06	74,74,74,74	0
35	NA	0	9116	1/1	0.93	0.16	51,51,51,51	0
37	SR	0	9566	1/1	0.93	0.07	97,97,97,97	0
37	SR	0	9459	1/1	0.93	0.07	93,93,93,93	0
35	NA	0	9135	1/1	0.93	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9120	1/1	0.93	0.17	59,59,59,59	0
33	MG	0	8082	1/1	0.93	0.36	80,80,80,80	0
33	MG	9	8095	1/1	0.93	0.26	46,46,46,46	0
33	MG	A	8066	1/1	0.93	0.18	57,57,57,57	0
37	SR	0	9500	1/1	0.93	1.21	196,196,196,196	0
33	MG	0	8043	1/1	0.93	0.07	56,56,56,56	0
33	MG	Y	8109	1/1	0.93	0.13	39,39,39,39	0
37	SR	H	9486	1/1	0.93	0.14	121,121,121,121	0
33	MG	0	8019	1/1	0.93	0.08	52,52,52,52	0
33	MG	0	8036	1/1	0.93	0.07	47,47,47,47	0
33	MG	0	8116	1/1	0.94	0.07	69,69,69,69	0
36	CL	0	9316	1/1	0.94	0.25	74,74,74,74	0
36	CL	0	9317	1/1	0.94	0.13	58,58,58,58	0
36	CL	L	9310	1/1	0.94	0.16	51,51,51,51	0
36	CL	M	9318	1/1	0.94	0.21	40,40,40,40	0
33	MG	0	8117	1/1	0.94	0.15	40,40,40,40	0
35	NA	0	9128	1/1	0.94	0.22	40,40,40,40	0
33	MG	0	8063	1/1	0.94	0.16	74,74,74,74	0
33	MG	0	8106	1/1	0.94	0.04	39,39,39,39	0
33	MG	0	8059	1/1	0.94	0.20	46,46,46,46	0
35	NA	0	9115	1/1	0.94	0.23	42,42,42,42	0
37	SR	0	9483	1/1	0.94	0.10	77,77,77,77	0
35	NA	0	9166	1/1	0.94	0.17	76,76,76,76	0
33	MG	0	8042	1/1	0.94	0.07	50,50,50,50	0
33	MG	0	8072	1/1	0.94	0.15	65,65,65,65	0
33	MG	0	8058	1/1	0.94	0.28	34,34,34,34	0
37	SR	F	9595	1/1	0.94	0.16	92,92,92,92	0
35	NA	D	9151	1/1	0.94	0.19	60,60,60,60	0
38	SPS	4	9701	23/23	0.94	0.17	39,45,57,60	0
33	MG	0	8114	1/1	0.94	0.21	74,74,74,74	0
33	MG	0	8096	1/1	0.94	0.07	37,37,37,37	0
33	MG	0	8091	1/1	0.95	0.08	55,55,55,55	0
33	MG	0	8084	1/1	0.95	0.56	107,107,107,107	0
33	MG	0	8026	1/1	0.95	0.18	25,25,25,25	0
35	NA	T	9143	1/1	0.95	0.08	37,37,37,37	0
37	SR	0	9568	1/1	0.95	0.04	86,86,86,86	0
33	MG	0	8110	1/1	0.95	0.25	40,40,40,40	0
35	NA	0	9131	1/1	0.95	0.15	51,51,51,51	0
37	SR	0	9489	1/1	0.95	0.09	101,101,101,101	0
35	NA	0	9170	1/1	0.95	0.27	92,92,92,92	0
36	CL	A	9309	1/1	0.95	0.18	70,70,70,70	0
36	CL	B	9319	1/1	0.95	0.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9106	1/1	0.95	0.32	39,39,39,39	0
37	SR	A	9497	1/1	0.95	0.09	99,99,99,99	0
33	MG	0	8030	1/1	0.95	0.09	38,38,38,38	0
36	CL	R	9306	1/1	0.95	0.11	45,45,45,45	0
37	SR	0	9515	1/1	0.95	0.09	109,109,109,109	0
36	CL	Y	9320	1/1	0.95	0.11	42,42,42,42	0
37	SR	0	9522	1/1	0.95	0.07	100,100,100,100	0
33	MG	0	8032	1/1	0.95	0.07	34,34,34,34	0
33	MG	0	8021	1/1	0.95	0.20	49,49,49,49	0
37	SR	0	9560	1/1	0.96	0.09	94,94,94,94	0
33	MG	0	8037	1/1	0.96	0.08	42,42,42,42	0
36	CL	J	9301	1/1	0.96	0.07	50,50,50,50	0
35	NA	0	9162	1/1	0.96	0.14	43,43,43,43	0
33	MG	0	8039	1/1	0.96	0.09	45,45,45,45	0
36	CL	N	9307	1/1	0.96	0.19	60,60,60,60	0
33	MG	0	8005	1/1	0.96	0.06	31,31,31,31	0
35	NA	0	9165	1/1	0.96	0.32	37,37,37,37	0
37	SR	0	9626	1/1	0.96	0.27	146,146,146,146	0
37	SR	9	9481	1/1	0.96	0.08	86,86,86,86	0
35	NA	0	9178	1/1	0.96	0.52	44,44,44,44	0
35	NA	0	9117	1/1	0.96	0.11	31,31,31,31	0
37	SR	A	9436	1/1	0.96	0.06	87,87,87,87	0
37	SR	0	9441	1/1	0.96	0.08	64,64,64,64	0
37	SR	0	9446	1/1	0.96	0.07	93,93,93,93	0
37	SR	0	9452	1/1	0.96	0.16	94,94,94,94	0
35	NA	0	9136	1/1	0.96	0.16	32,32,32,32	0
35	NA	0	9156	1/1	0.96	0.38	57,57,57,57	0
37	SR	0	9467	1/1	0.96	0.11	73,73,73,73	0
33	MG	0	8025	1/1	0.96	0.30	19,19,19,19	0
33	MG	T	8073	1/1	0.96	0.11	34,34,34,34	0
33	MG	0	8020	1/1	0.97	0.19	37,37,37,37	0
33	MG	0	8002	1/1	0.97	0.12	33,33,33,33	0
35	NA	M	9147	1/1	0.97	0.15	33,33,33,33	0
35	NA	Q	9148	1/1	0.97	0.10	48,48,48,48	0
35	NA	R	9137	1/1	0.97	0.10	23,23,23,23	0
37	SR	0	9426	1/1	0.97	0.08	72,72,72,72	0
37	SR	0	9433	1/1	0.97	0.17	74,74,74,74	0
37	SR	0	9534	1/1	0.97	0.12	113,113,113,113	0
35	NA	R	9186	1/1	0.97	0.15	75,75,75,75	0
37	SR	0	9545	1/1	0.97	0.08	84,84,84,84	0
35	NA	0	9118	1/1	0.97	0.20	43,43,43,43	0
35	NA	0	9130	1/1	0.97	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
37	SR	0	9454	1/1	0.97	0.14	79,79,79,79	0
33	MG	4	8118	1/1	0.97	0.22	29,29,29,29	0
37	SR	0	9461	1/1	0.97	0.04	86,86,86,86	0
37	SR	0	9464	1/1	0.97	0.07	80,80,80,80	0
36	CL	0	9303	1/1	0.97	0.14	47,47,47,47	0
36	CL	0	9311	1/1	0.97	0.14	66,66,66,66	0
36	CL	0	9313	1/1	0.97	0.08	51,51,51,51	0
37	SR	0	9477	1/1	0.97	0.12	79,79,79,79	0
37	SR	0	9629	1/1	0.97	0.09	73,73,73,73	0
37	SR	0	9478	1/1	0.97	0.08	72,72,72,72	0
37	SR	0	9480	1/1	0.97	0.05	83,83,83,83	0
36	CL	0	9315	1/1	0.97	0.13	58,58,58,58	0
33	MG	0	8070	1/1	0.97	0.15	26,26,26,26	0
35	NA	0	9123	1/1	0.97	0.12	50,50,50,50	0
36	CL	0	9322	1/1	0.97	0.21	53,53,53,53	0
33	MG	0	8080	1/1	0.97	0.18	46,46,46,46	0
33	MG	B	8056	1/1	0.97	0.22	46,46,46,46	0
35	NA	0	9138	1/1	0.97	0.11	56,56,56,56	0
37	SR	0	9504	1/1	0.97	0.10	92,92,92,92	0
35	NA	0	9105	1/1	0.97	0.06	36,36,36,36	0
35	NA	C	9104	1/1	0.97	0.17	26,26,26,26	0
37	SR	0	9444	1/1	0.98	0.12	52,52,52,52	0
37	SR	0	9445	1/1	0.98	0.12	62,62,62,62	0
33	MG	0	8028	1/1	0.98	0.12	31,31,31,31	0
33	MG	0	8029	1/1	0.98	0.26	22,22,22,22	0
33	MG	0	8012	1/1	0.98	0.25	26,26,26,26	0
35	NA	0	9160	1/1	0.98	0.17	45,45,45,45	0
33	MG	0	8031	1/1	0.98	0.09	48,48,48,48	0
36	CL	J	9302	1/1	0.98	0.06	54,54,54,54	0
36	CL	J	9321	1/1	0.98	0.14	65,65,65,65	0
37	SR	0	9466	1/1	0.98	0.05	95,95,95,95	0
33	MG	0	8004	1/1	0.98	0.09	24,24,24,24	0
33	MG	0	8079	1/1	0.98	0.11	29,29,29,29	0
37	SR	0	9473	1/1	0.98	0.06	77,77,77,77	0
35	NA	0	9108	1/1	0.98	0.10	31,31,31,31	0
36	CL	O	9308	1/1	0.98	0.14	56,56,56,56	0
33	MG	0	8015	1/1	0.98	0.09	29,29,29,29	0
33	MG	0	8001	1/1	0.98	0.23	17,17,17,17	0
33	MG	K	8069	1/1	0.98	0.18	20,20,20,20	0
37	SR	0	9405	1/1	0.98	0.04	81,81,81,81	0
37	SR	0	9488	1/1	0.98	0.15	80,80,80,80	0
37	SR	0	9421	1/1	0.98	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9422	1/1	0.98	0.13	57,57,57,57	0
37	SR	0	9495	1/1	0.98	0.12	90,90,90,90	0
37	SR	A	9437	1/1	0.98	0.11	70,70,70,70	0
33	MG	0	8038	1/1	0.98	0.24	16,16,16,16	0
36	CL	0	9314	1/1	0.98	0.17	52,52,52,52	0
37	SR	0	9427	1/1	0.98	0.15	55,55,55,55	0
37	SR	0	9432	1/1	0.98	0.16	65,65,65,65	0
33	MG	0	8009	1/1	0.98	0.08	31,31,31,31	0
37	SR	S	9470	1/1	0.98	0.16	98,98,98,98	0
37	SR	0	9438	1/1	0.98	0.11	66,66,66,66	0
37	SR	0	9509	1/1	0.98	0.14	86,86,86,86	0
33	MG	0	8067	1/1	0.98	0.14	35,35,35,35	0
37	SR	0	9434	1/1	0.99	0.17	61,61,61,61	0
37	SR	0	9498	1/1	0.99	0.07	65,65,65,65	0
37	SR	0	9435	1/1	0.99	0.10	71,71,71,71	0
33	MG	0	8017	1/1	0.99	0.14	18,18,18,18	0
37	SR	0	9440	1/1	0.99	0.08	60,60,60,60	0
33	MG	0	8013	1/1	0.99	0.40	10,10,10,10	0
37	SR	0	9442	1/1	0.99	0.15	63,63,63,63	0
37	SR	0	9443	1/1	0.99	0.13	62,62,62,62	0
37	SR	0	9407	1/1	0.99	0.20	50,50,50,50	0
37	SR	0	9408	1/1	0.99	0.22	48,48,48,48	0
37	SR	0	9410	1/1	0.99	0.20	46,46,46,46	0
37	SR	0	9447	1/1	0.99	0.14	62,62,62,62	0
37	SR	0	9448	1/1	0.99	0.10	64,64,64,64	0
37	SR	0	9449	1/1	0.99	0.11	61,61,61,61	0
37	SR	0	9450	1/1	0.99	0.08	63,63,63,63	0
37	SR	0	9451	1/1	0.99	0.19	57,57,57,57	0
37	SR	0	9411	1/1	0.99	0.20	49,49,49,49	0
37	SR	0	9453	1/1	0.99	0.11	76,76,76,76	0
37	SR	0	9412	1/1	0.99	0.15	51,51,51,51	0
37	SR	0	9455	1/1	0.99	0.10	66,66,66,66	0
37	SR	0	9456	1/1	0.99	0.13	69,69,69,69	0
37	SR	0	9457	1/1	0.99	0.14	50,50,50,50	0
37	SR	0	9413	1/1	0.99	0.17	50,50,50,50	0
37	SR	0	9414	1/1	0.99	0.15	56,56,56,56	0
37	SR	0	9462	1/1	0.99	0.15	67,67,67,67	0
37	SR	0	9416	1/1	0.99	0.15	48,48,48,48	0
37	SR	0	9417	1/1	0.99	0.14	58,58,58,58	0
37	SR	0	9420	1/1	0.99	0.17	74,74,74,74	0
36	CL	K	9312	1/1	0.99	0.10	45,45,45,45	0
33	MG	0	8003	1/1	0.99	0.13	24,24,24,24	0

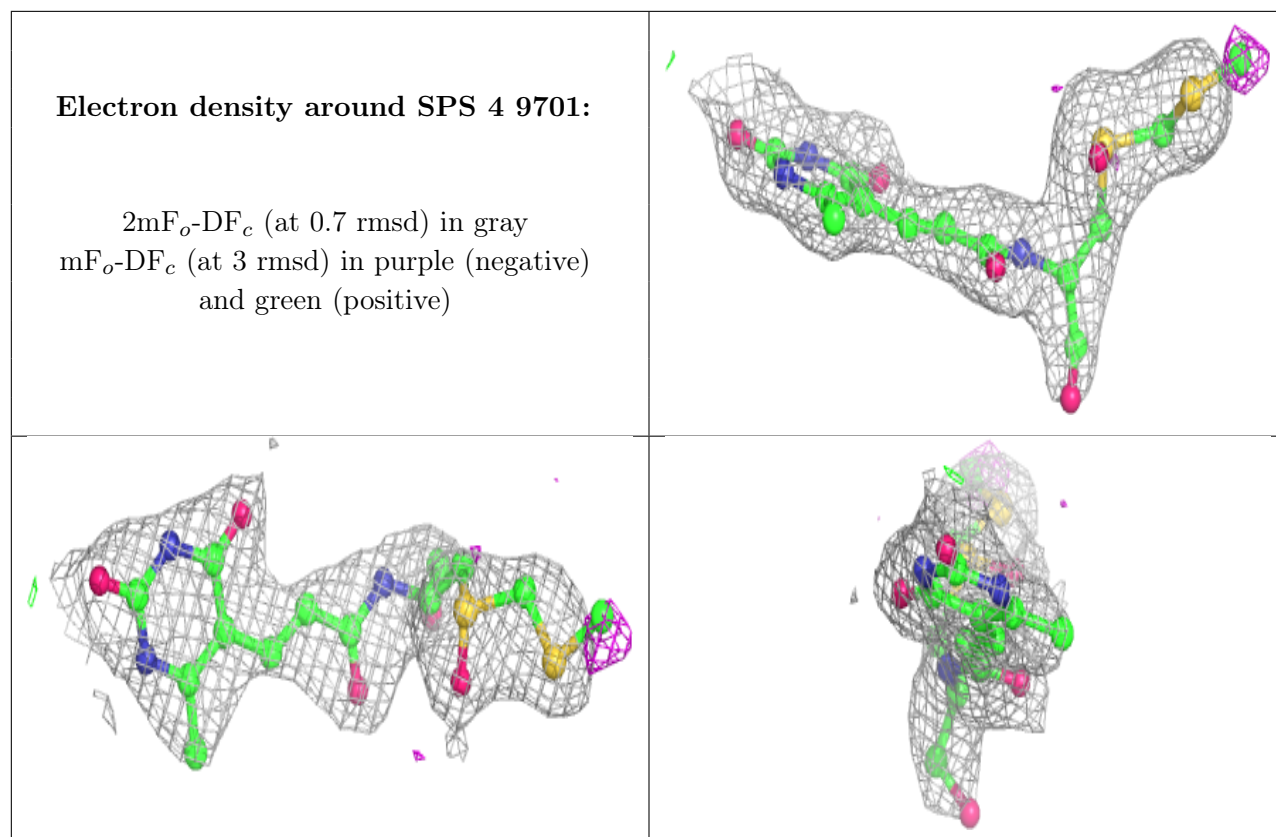
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9469	1/1	0.99	0.07	88,88,88,88	0
37	SR	0	9424	1/1	0.99	0.21	49,49,49,49	0
37	SR	0	9474	1/1	0.99	0.11	68,68,68,68	0
37	SR	0	9475	1/1	0.99	0.09	80,80,80,80	0
33	MG	0	8044	1/1	0.99	0.06	35,35,35,35	0
33	MG	0	8074	1/1	0.99	0.20	15,15,15,15	0
37	SR	B	9458	1/1	0.99	0.13	66,66,66,66	0
36	CL	0	9305	1/1	0.99	0.08	58,58,58,58	0
37	SR	0	9428	1/1	0.99	0.12	51,51,51,51	0
37	SR	0	9429	1/1	0.99	0.15	67,67,67,67	0
37	SR	L	9409	1/1	0.99	0.14	46,46,46,46	0
37	SR	R	9418	1/1	0.99	0.17	58,58,58,58	0
37	SR	0	9430	1/1	0.99	0.17	48,48,48,48	0
37	SR	1	9419	1/1	0.99	0.18	47,47,47,47	0
37	SR	1	9460	1/1	0.99	0.14	52,52,52,52	0
37	SR	3	9439	1/1	0.99	0.03	79,79,79,79	0
37	SR	0	9431	1/1	0.99	0.16	57,57,57,57	0
33	MG	0	8008	1/1	0.99	0.18	15,15,15,15	0
39	CD	U	9201	1/1	0.99	0.11	61,61,61,61	0
33	MG	0	8027	1/1	0.99	0.24	31,31,31,31	0
39	CD	1	9202	1/1	0.99	0.08	58,58,58,58	0
39	CD	3	9204	1/1	0.99	0.02	70,70,70,70	0
37	SR	0	9423	1/1	1.00	0.12	56,56,56,56	0
37	SR	0	9415	1/1	1.00	0.16	57,57,57,57	0
37	SR	0	9406	1/1	1.00	0.22	45,45,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.