



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 5, 2023 – 11:38 PM EST

PDB ID : 1M90  
Title : Co-crystal structure of CCA-Phe-caproic acid-biotin and sparsomycin bound to the 50S ribosomal subunit  
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2002-07-26  
Resolution : 2.80 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

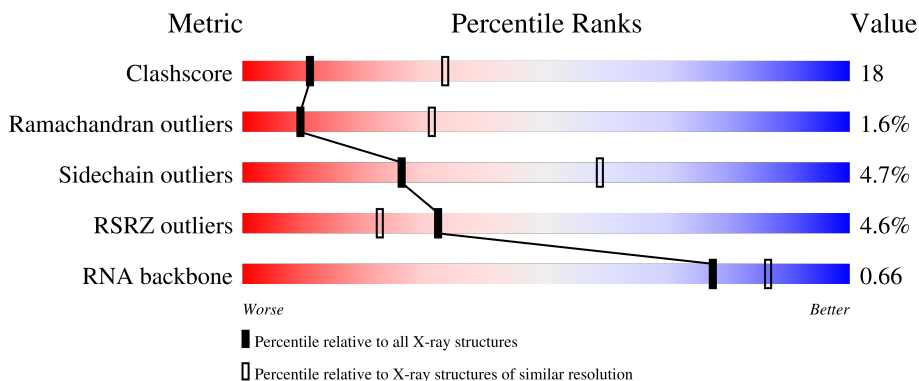
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.




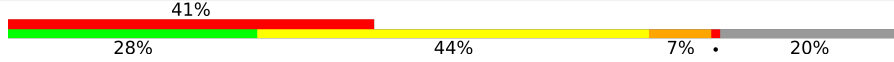


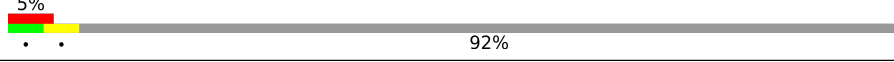
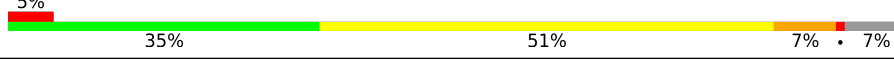
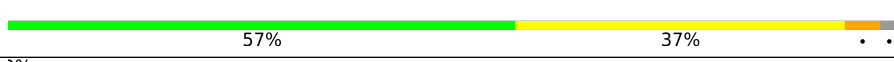
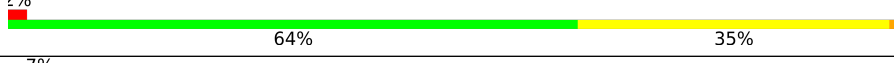
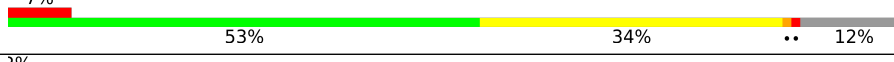

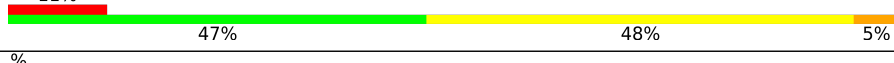
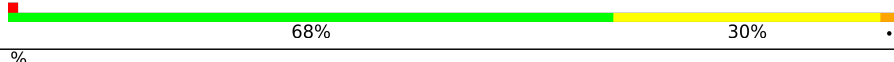

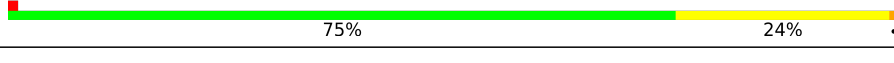
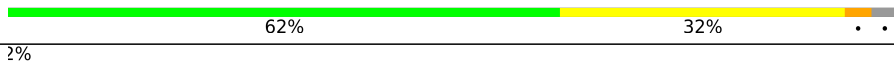


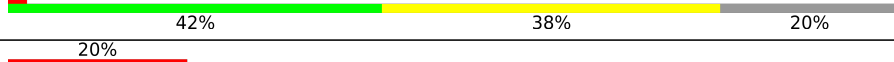



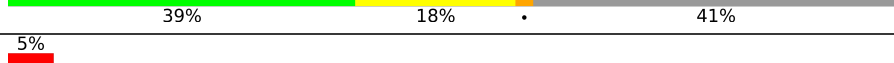



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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	A	2922	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div>
2	B	122	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div>
3	5	3	<div style="display: flex; align-items: center;"> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: red;"></div> </div>
4	C	239	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>
5	D	337	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange;"></div> </div>

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Mol	Chain	Length	Quality of chain
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	
30	3	48	

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Mol	Chain	Length	Quality of chain
31	4	92	 % 61% 35%

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	A	8024	-	-	-	X
33	NA	A	8352	-	-	-	X
33	NA	A	8384	-	-	-	X
33	NA	A	8385	-	-	-	X
33	NA	B	8351	-	-	-	X
33	NA	S	8386	-	-	-	X
33	NA	T	8312	-	-	-	X

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98611 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2754	59017	26346	10878	19048	2745	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	conflict	GB 3377779

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

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.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L2.

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 RIBOSOMAL PROTEIN L3.

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 RIBOSOMAL PROTEIN L4.

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 RIBOSOMAL PROTEIN L5.

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 RIBOSOMAL PROTEIN L6.

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 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 RIBOSOMAL PROTEIN L10.

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 RIBOSOMAL PROTEIN L10E.

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 RIBOSOMAL PROTEIN L13.

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 RIBOSOMAL PROTEIN L14.

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 RIBOSOMAL PROTEIN L15.

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 RIBOSOMAL PROTEIN L15E.

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 RIBOSOMAL PROTEIN L18.

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 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 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 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 RIBOSOMAL PROTEIN L22.

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 RIBOSOMAL PROTEIN L23.

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 RIBOSOMAL PROTEIN L24.

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 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 RIBOSOMAL PROTEIN L29.

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 RIBOSOMAL PROTEIN L30.



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 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 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 RIBOSOMAL PROTEIN L37Ae.

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 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 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 RIBOSOMAL PROTEIN L44E.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	111	Total	Mg	0	0
			111	111		
32	B	1	Total	Mg	0	0
			1	1		
32	5	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
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 SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	A	73	Total	Na	0	0
			73	73		
33	B	2	Total	Na	0	0
			2	2		
33	C	1	Total	Na	0	0
			1	1		
33	E	1	Total	Na	0	0
			1	1		
33	J	1	Total	Na	0	0
			1	1		
33	K	1	Total	Na	0	0
			1	1		
33	M	1	Total	Na	0	0
			1	1		
33	N	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	R	1	Total 1	Na 1	0	0
33	S	2	Total 2	Na 2	0	0
33	T	1	Total 1	Na 1	0	0
33	U	1	Total 1	Na 1	0	0

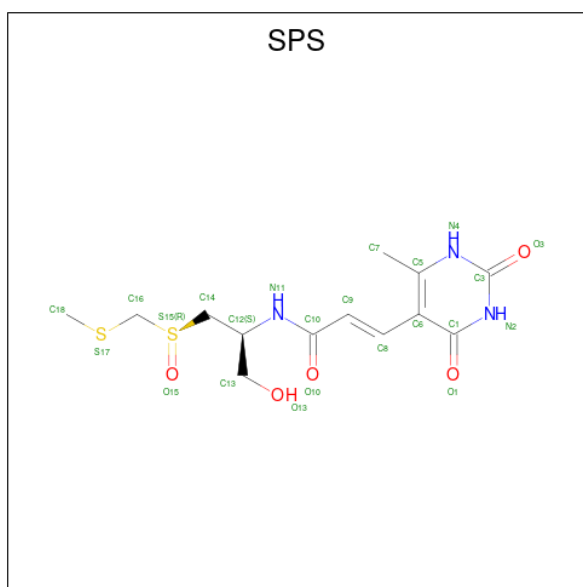
- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

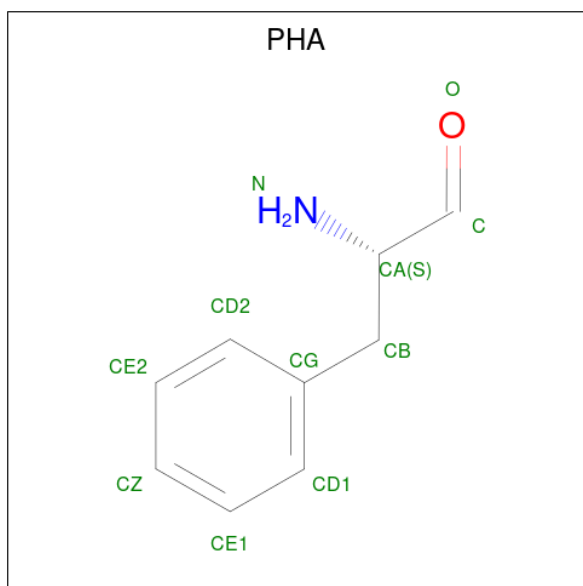
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	10	Total 10	Cl 10	0	0
35	C	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	P	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	Z	1	Total 1	Cl 1	0	0
35	4	1	Total 1	Cl 1	0	0

- Molecule 36 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>).



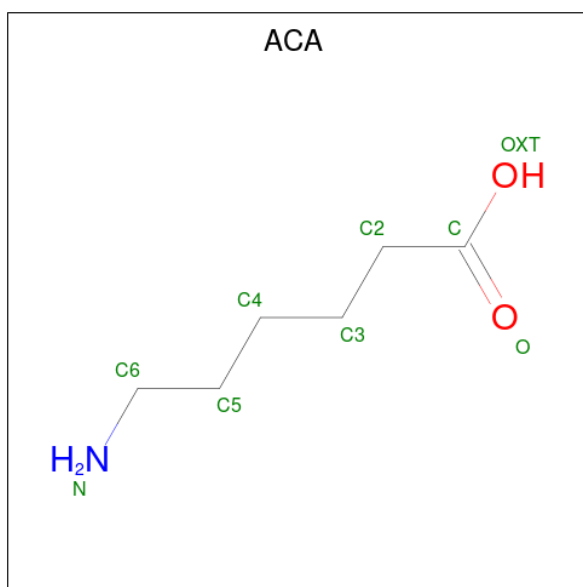
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
36	5	1	23	13	3	5	2	0	0

- Molecule 37 is PHENYLALANINAL (three-letter code: PHA) (formula:  $C_9H_{11}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
37	5	1	11	9	1	1	0	0

- Molecule 38 is 6-AMINOHEXANOIC ACID (three-letter code: ACA) (formula:  $C_6H_{13}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	5	1	Total	C	N	O	0	0
			8	6	1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	P	1	Total	Cd	0	0
			1	1		
39	V	1	Total	Cd	0	0
			1	1		
39	1	1	Total	Cd	0	0
			1	1		
39	2	1	Total	Cd	0	0
			1	1		
39	4	1	Total	Cd	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	5920	Total	O	0	0
			5920	5920		
40	B	136	Total	O	0	0
			136	136		
40	5	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	C	119	Total 119	O 119	0	0
40	D	142	Total 142	O 142	0	0
40	E	172	Total 172	O 172	0	0
40	F	51	Total 51	O 51	0	0
40	G	44	Total 44	O 44	0	0
40	H	28	Total 28	O 28	0	0
40	I	21	Total 21	O 21	0	0
40	J	75	Total 75	O 75	0	0
40	K	56	Total 56	O 56	0	0
40	L	61	Total 61	O 61	0	0
40	M	86	Total 86	O 86	0	0
40	N	125	Total 125	O 125	0	0
40	O	69	Total 69	O 69	0	0
40	P	43	Total 43	O 43	0	0
40	Q	67	Total 67	O 67	0	0
40	R	49	Total 49	O 49	0	0
40	S	83	Total 83	O 83	0	0
40	T	35	Total 35	O 35	0	0
40	U	37	Total 37	O 37	0	0
40	V	24	Total 24	O 24	0	0
40	W	16	Total 16	O 16	0	0

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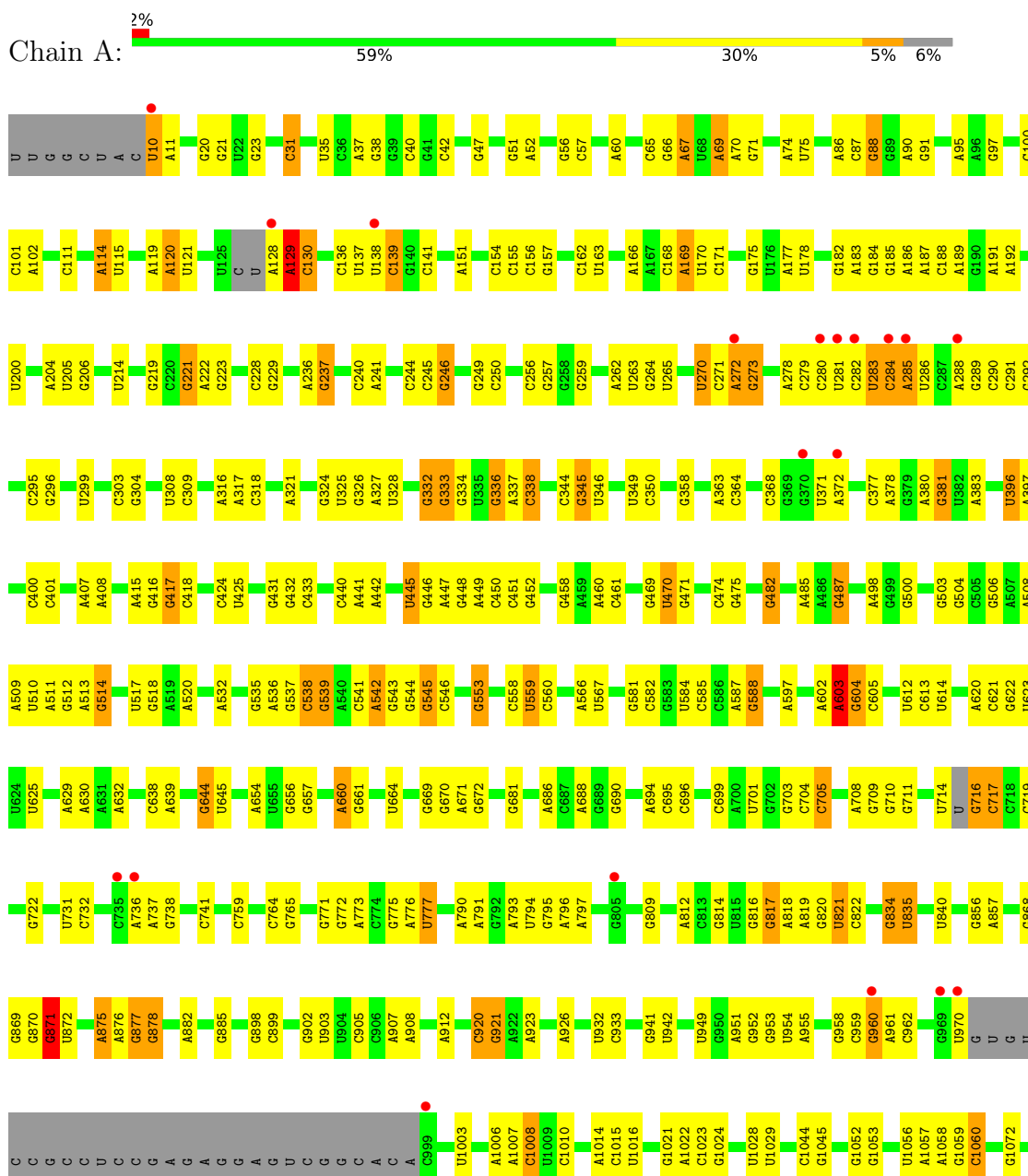
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
40	X	71	Total 71	O 71	0	0
40	Y	31	Total 31	O 31	0	0
40	Z	92	Total 92	O 92	0	0
40	1	36	Total 36	O 36	0	0
40	2	55	Total 55	O 55	0	0
40	3	40	Total 40	O 40	0	0
40	4	73	Total 73	O 73	0	0

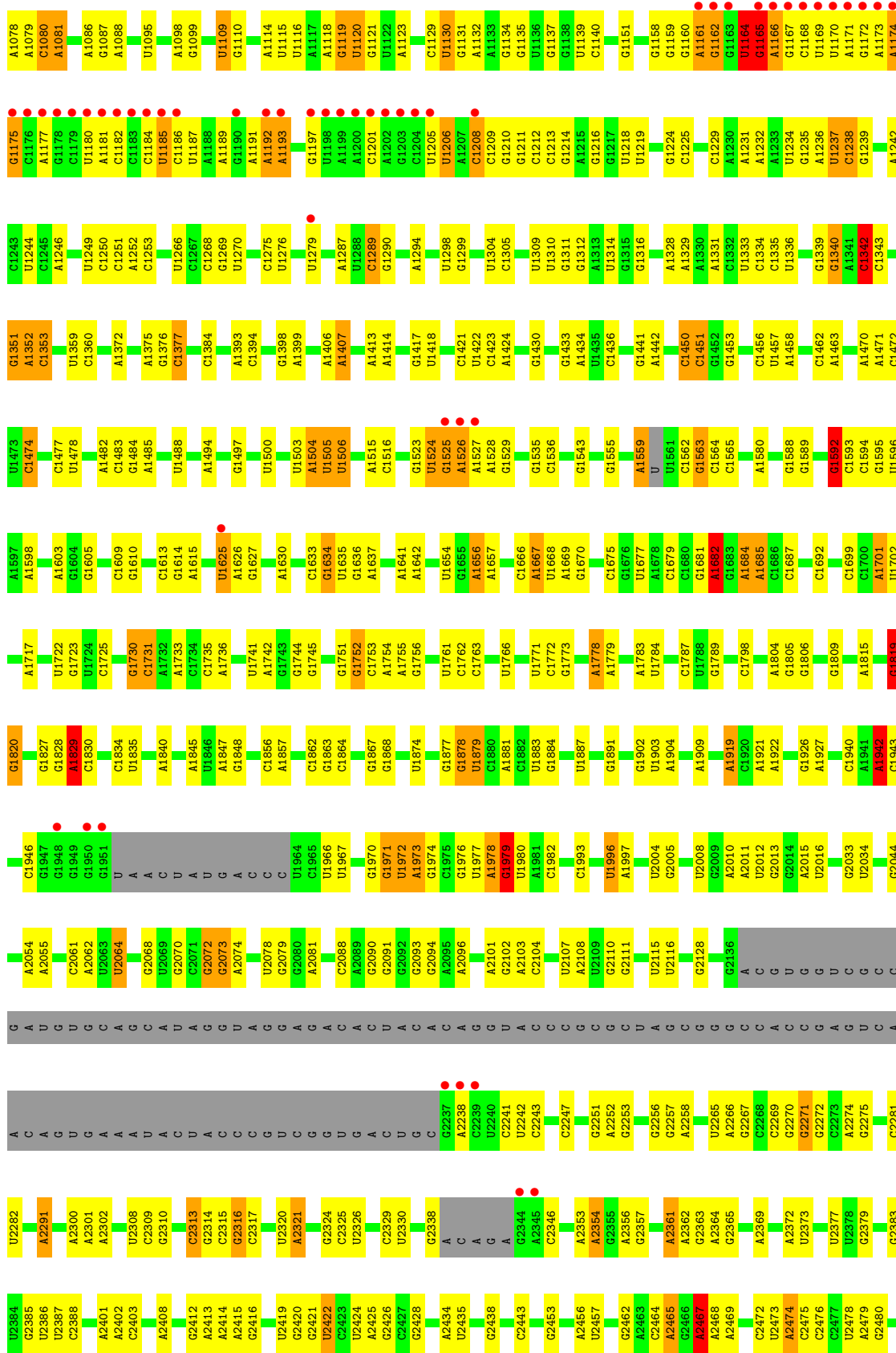
### 3 Residue-property plots i

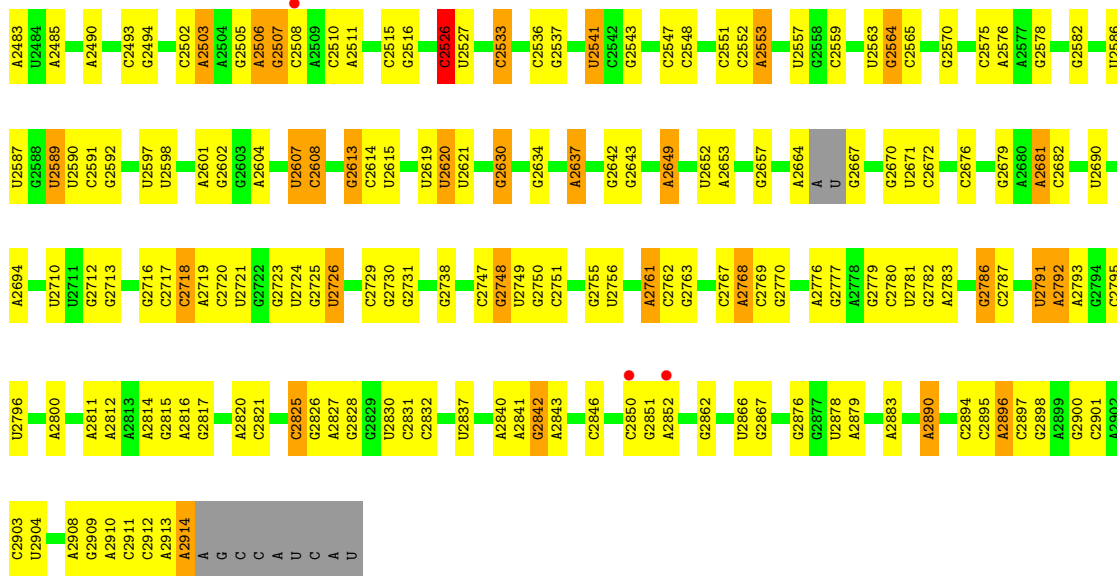
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 RRNA

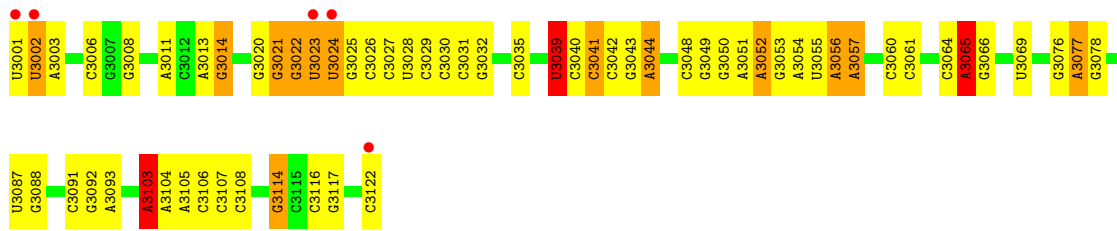








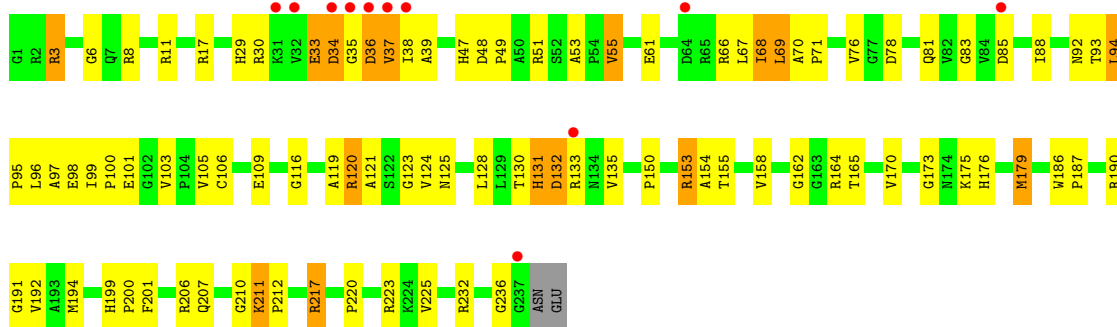
• Molecule 2: 5S RRNA



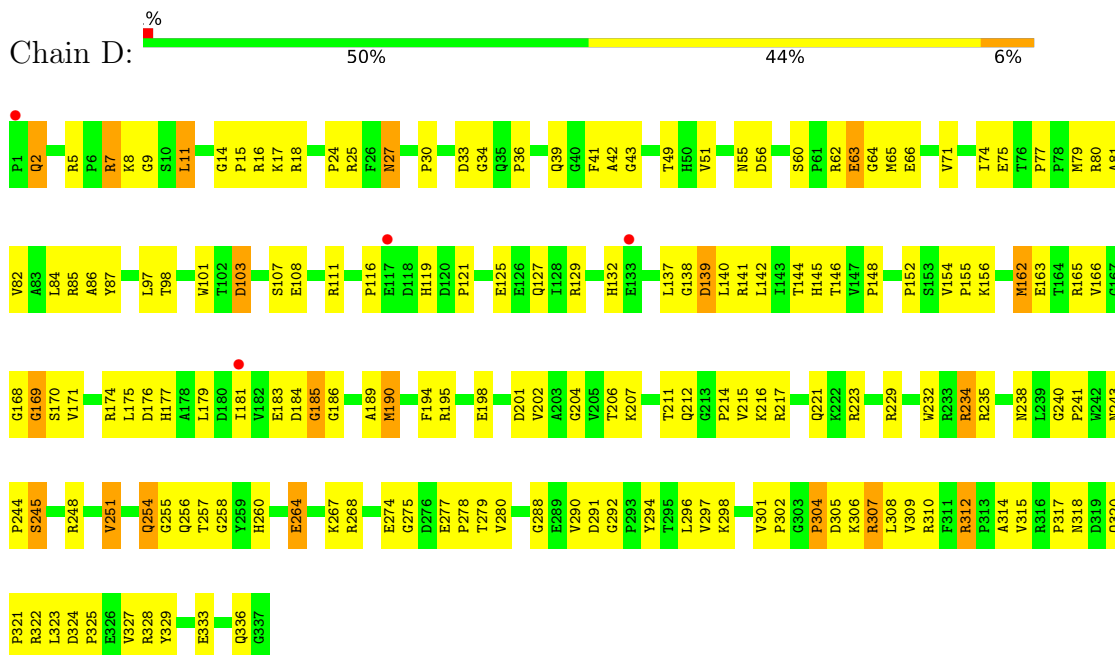
• Molecule 3: CCA



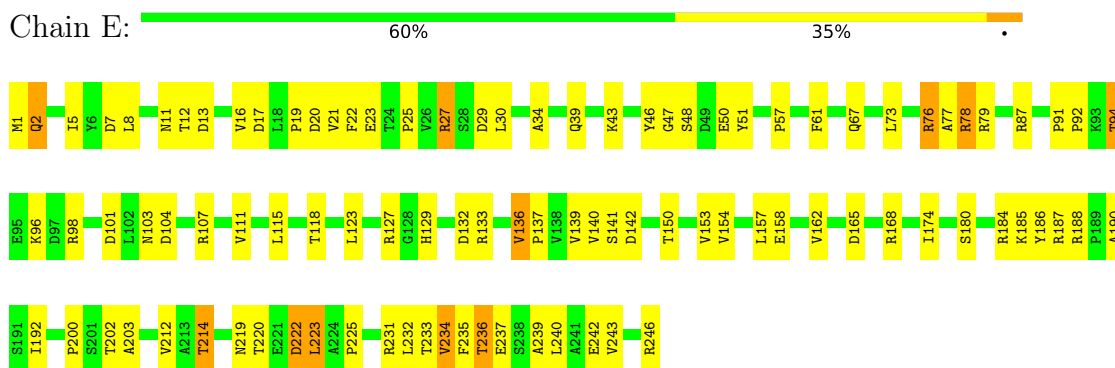
• Molecule 4: RIBOSOMAL PROTEIN L2



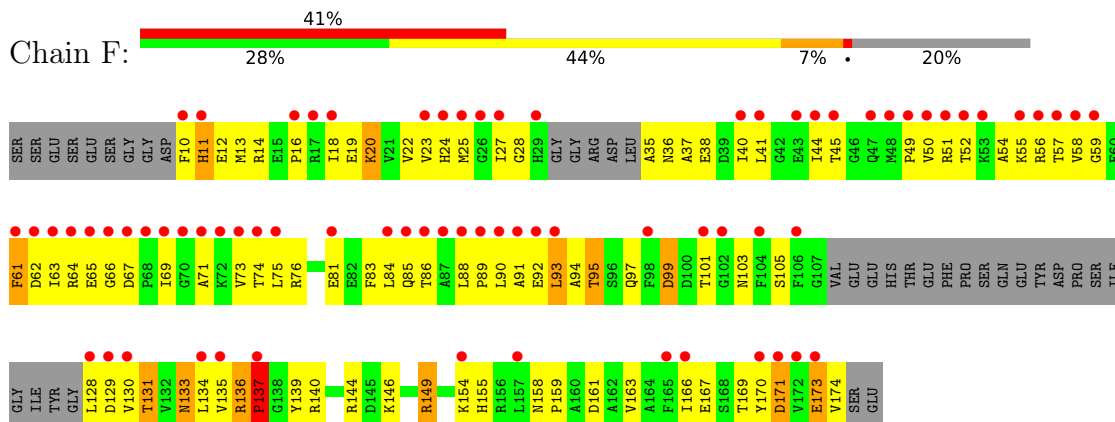
- Molecule 5: RIBOSOMAL PROTEIN L3



- Molecule 6: RIBOSOMAL PROTEIN L4

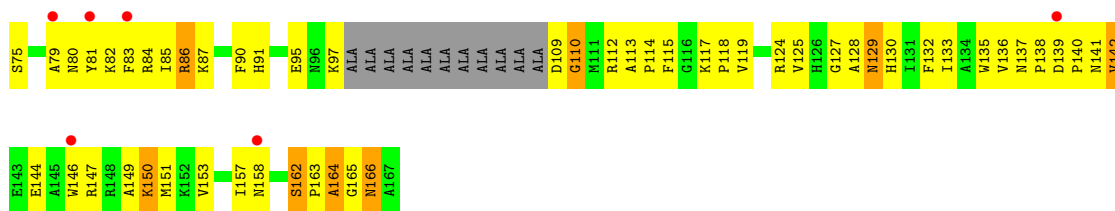


- Molecule 7: RIBOSOMAL PROTEIN L5



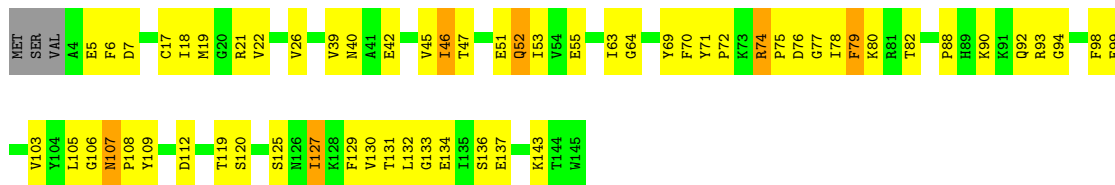
- Molecule 8: RIBOSOMAL PROTEIN L6





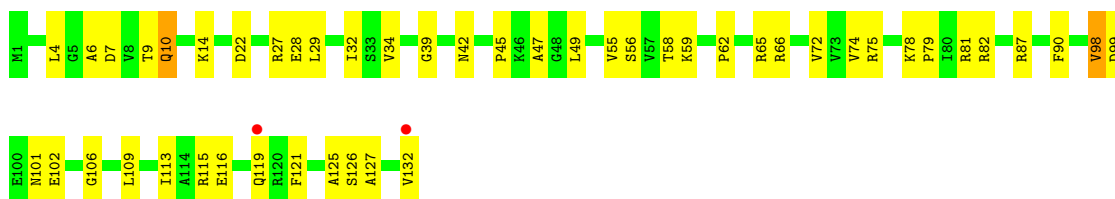
● Molecule 12: RIBOSOMAL PROTEIN L13

Chain K: 57% 37%



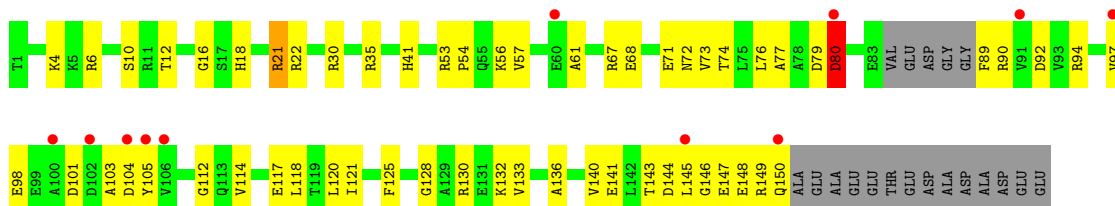
● Molecule 13: RIBOSOMAL PROTEIN L14

Chain L: 2% 64% 35%



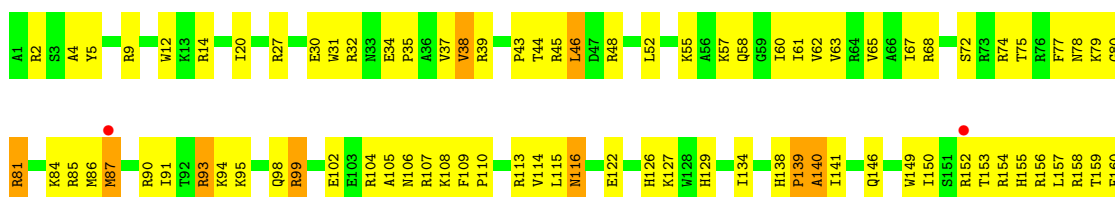
● Molecule 14: RIBOSOMAL PROTEIN L15

Chain M: 7% 53% 34% 12%



● Molecule 15: RIBOSOMAL PROTEIN L15E

Chain N: 2% 46% 49% 5%





• Molecule 16: RIBOSOMAL PROTEIN L18



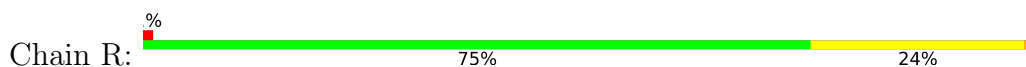
• Molecule 17: RIBOSOMAL PROTEIN L18E



• Molecule 18: RIBOSOMAL PROTEIN L19E

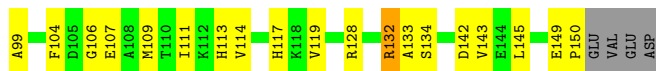


• Molecule 19: RIBOSOMAL PROTEIN L21E



• Molecule 20: RIBOSOMAL PROTEIN L22

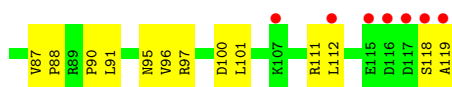
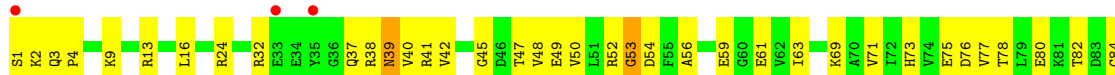




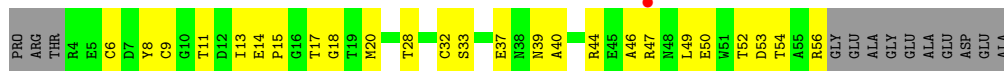
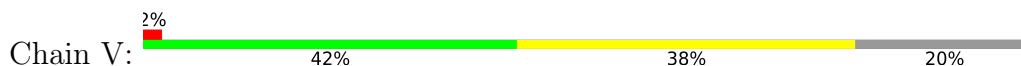
- Molecule 21: RIBOSOMAL PROTEIN L23



- Molecule 22: RIBOSOMAL PROTEIN L24



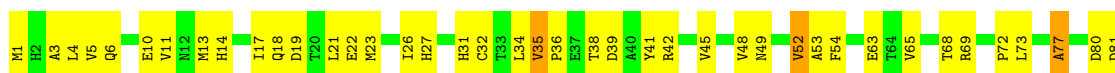
- Molecule 23: RIBOSOMAL PROTEIN L24E



- Molecule 24: RIBOSOMAL PROTEIN L29



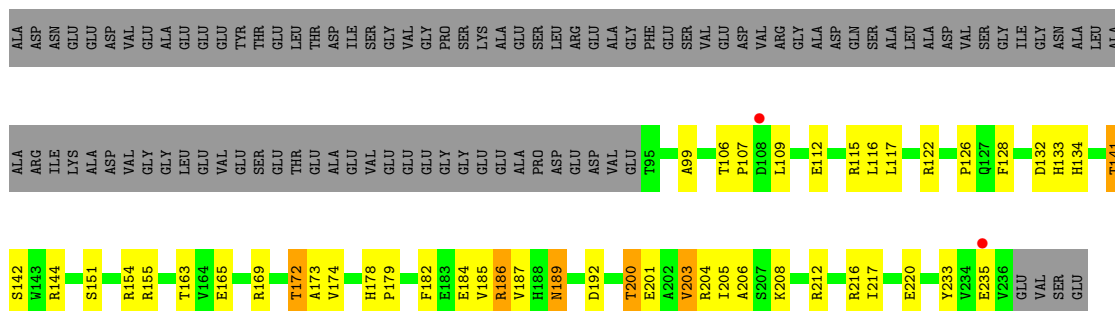
- Molecule 25: RIBOSOMAL PROTEIN L30



- Molecule 26: RIBOSOMAL PROTEIN L31E



- Molecule 27: RIBOSOMAL PROTEIN L32E



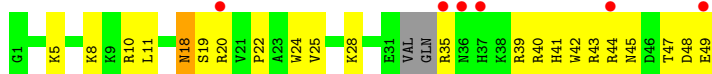
- Molecule 28: RIBOSOMAL PROTEIN L37Ae



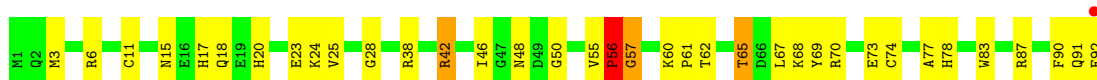
- Molecule 29: RIBOSOMAL PROTEIN L37E



- Molecule 30: RIBOSOMAL PROTEIN L39E



- Molecule 31: RIBOSOMAL PROTEIN L44E





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.66Å 299.77Å 573.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 49.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (20.00-2.80) 94.4 (49.96-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.181 , 0.222 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	98611	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 1.50% 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: CD, SPS, K, ACA, PHA, NA, CL, MG

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	0.42	1/66076 (0.0%)	0.70	27/103052 (0.0%)
2	B	0.50	0/2905	0.79	4/4528 (0.1%)
3	5	0.74	0/65	1.17	1/99 (1.0%)
4	C	0.34	0/1787	0.66	0/2409
5	D	0.34	0/2689	0.65	0/3652
6	E	0.40	0/1883	0.66	0/2551
7	F	0.33	0/1111	0.60	0/1498
8	G	0.34	0/1382	0.59	0/1880
9	H	0.33	0/896	0.58	0/1219
10	I	0.27	0/241	0.47	0/324
11	J	0.39	0/1246	0.75	2/1686 (0.1%)
12	K	0.37	0/1135	0.61	0/1530
13	L	0.35	0/1003	0.67	0/1351
14	M	0.34	0/1126	0.67	0/1504
15	N	0.41	0/1633	0.70	1/2180 (0.0%)
16	O	0.31	0/1473	0.64	0/1999
17	P	0.38	0/873	0.63	0/1181
18	Q	0.37	0/1143	0.56	0/1521
19	R	0.38	0/748	0.67	0/1005
20	S	0.38	0/1172	0.67	0/1578
21	T	0.34	0/648	0.60	0/875
22	U	0.32	0/957	0.63	0/1289
23	V	0.35	0/417	0.57	0/562
24	W	0.32	0/502	0.56	0/675
25	X	0.36	0/1218	0.64	0/1655
26	Y	0.36	0/664	0.61	0/895
27	Z	0.39	0/1146	0.67	0/1536
28	1	0.39	0/575	0.71	0/763
29	2	0.44	0/437	0.67	0/578
30	3	0.34	0/398	0.56	0/527
31	4	0.40	0/771	0.62	0/1024
All	All	0.41	1/98320 (0.0%)	0.69	35/147126 (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	1	58
2	B	0	3
All	All	1	61

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2474	A	C5-C6	-5.43	1.36	1.41

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-17.46	66.80	105.20
1	A	1164	U	OP2-P-O3'	-16.54	68.82	105.20
1	A	1563	G	C2'-C3'-O3'	9.62	130.67	109.50
1	A	1979	G	C2'-C3'-O3'	7.74	126.52	109.50
1	A	1942	A	C5'-C4'-C3'	7.39	127.82	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 61 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	G	Sidechain
1	A	246	G	Sidechain
1	A	270	U	Sidechain
1	A	332	G	Sidechain
1	A	333	G	Sidechain

## 5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29805	894	0
2	B	2600	0	1326	73	0
3	5	59	0	34	2	0
4	C	1754	0	1763	129	0
5	D	2624	0	2533	176	0
6	E	1858	0	1816	114	0
7	F	1094	0	1085	127	0
8	G	1357	0	1266	77	0
9	H	885	0	854	62	0
10	I	240	0	231	21	0
11	J	1215	0	1215	152	0
12	K	1119	0	1098	67	0
13	L	993	0	1027	55	0
14	M	1114	0	1072	61	0
15	N	1605	0	1676	159	0
16	O	1444	0	1401	128	0
17	P	864	0	873	41	0
18	Q	1133	0	1127	49	0
19	R	734	0	728	21	0
20	S	1149	0	1122	65	0
21	T	641	0	605	19	0
22	U	949	0	923	48	0
23	V	410	0	364	32	0
24	W	499	0	511	34	0
25	X	1195	0	1137	101	0
26	Y	654	0	653	47	0
27	Z	1130	0	1133	61	0
28	1	563	0	597	59	0
29	2	430	0	426	24	0
30	3	393	0	406	28	0
31	4	755	0	728	36	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	5	1	0	0	0	0
32	A	111	0	0	0	0
32	B	1	0	0	0	0
32	C	1	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	73	0	0	0	0
33	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	1	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
33	U	1	0	0	0	0
34	A	2	0	0	0	0
35	4	1	0	0	0	0
35	A	10	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	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	23	0	19	4	0
37	5	11	0	8	0	0
38	5	8	0	6	0	0
39	1	1	0	0	0	0
39	2	1	0	0	0	0
39	4	1	0	0	0	0
39	P	1	0	0	0	0
39	V	1	0	0	0	0
40	1	36	0	0	8	0
40	2	55	0	0	3	0
40	3	40	0	0	4	0
40	4	73	0	0	10	0
40	5	1	0	0	0	0
40	A	5920	0	0	193	0
40	B	136	0	0	11	0
40	C	119	0	0	23	0
40	D	142	0	0	30	0
40	E	172	0	0	27	0
40	F	51	0	0	23	0
40	G	44	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	H	28	0	0	8	0
40	I	21	0	0	6	0
40	J	75	0	0	23	0
40	K	56	0	0	5	0
40	L	61	0	0	16	0
40	M	86	0	0	19	0
40	N	125	0	0	21	0
40	O	69	0	0	17	0
40	P	43	0	0	7	0
40	Q	67	0	0	1	0
40	R	49	0	0	3	0
40	S	83	0	0	11	0
40	T	35	0	0	5	0
40	U	37	0	0	4	0
40	V	24	0	0	5	0
40	W	16	0	0	2	0
40	X	71	0	0	12	0
40	Y	31	0	0	5	0
40	Z	92	0	0	14	0
All	All	98611	0	59568	2699	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 18.

The worst 5 of 2699 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	1.04	1.16
1:A:1160:G:H5'	1:A:1161:A:H5'	1.22	1.15
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.63	1.13
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.30	1.12
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.31	1.12

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%)	209 (89%)	21 (9%)	5 (2%)	7	23
5	D	335/337 (99%)	303 (90%)	25 (8%)	7 (2%)	7	23
6	E	244/246 (99%)	218 (89%)	25 (10%)	1 (0%)	34	66
7	F	134/176 (76%)	98 (73%)	28 (21%)	8 (6%)	1	4
8	G	170/177 (96%)	159 (94%)	10 (6%)	1 (1%)	25	56
9	H	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	5	18
10	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	J	152/167 (91%)	133 (88%)	13 (9%)	6 (4%)	3	10
12	K	140/145 (97%)	126 (90%)	11 (8%)	3 (2%)	7	23
13	L	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	10	33
14	M	141/164 (86%)	120 (85%)	19 (14%)	2 (1%)	11	34
15	N	192/194 (99%)	174 (91%)	16 (8%)	2 (1%)	15	44
16	O	184/186 (99%)	167 (91%)	11 (6%)	6 (3%)	4	13
17	P	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
18	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	22	53
19	R	93/95 (98%)	85 (91%)	8 (9%)	0	100	100
20	S	148/154 (96%)	140 (95%)	7 (5%)	1 (1%)	22	53
21	T	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
22	U	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	17	46
23	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	4	13
25	X	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	12	36
26	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	5	19
27	Z	140/240 (58%)	139 (99%)	1 (1%)	0	100	100
28	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	11	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	2	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	85 (94%)	3 (3%)	2 (2%)	6	22
All	All	3633/4235 (86%)	3313 (91%)	262 (7%)	58 (2%)	9	31

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	20	LYS
7	F	93	LEU
7	F	95	THR
7	F	173	GLU

### 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	38
5	D	282/282 (100%)	264 (94%)	18 (6%)	17	45
6	E	193/193 (100%)	177 (92%)	16 (8%)	11	32
7	F	117/147 (80%)	109 (93%)	8 (7%)	16	42
8	G	152/155 (98%)	148 (97%)	4 (3%)	46	79
9	H	92/92 (100%)	91 (99%)	1 (1%)	73	92
10	I	27/283 (10%)	27 (100%)	0	100	100
11	J	122/122 (100%)	110 (90%)	12 (10%)	8	24
12	K	118/121 (98%)	109 (92%)	9 (8%)	13	36
13	L	106/106 (100%)	103 (97%)	3 (3%)	43	77
14	M	112/126 (89%)	109 (97%)	3 (3%)	44	78
15	N	166/166 (100%)	157 (95%)	9 (5%)	22	53
16	O	149/149 (100%)	144 (97%)	5 (3%)	37	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	93/93 (100%)	91 (98%)	2 (2%)	52	83
18	Q	113/116 (97%)	110 (97%)	3 (3%)	44	78
19	R	79/79 (100%)	75 (95%)	4 (5%)	24	55
20	S	117/121 (97%)	113 (97%)	4 (3%)	37	71
21	T	71/73 (97%)	71 (100%)	0	100	100
22	U	105/105 (100%)	104 (99%)	1 (1%)	76	93
23	V	44/52 (85%)	44 (100%)	0	100	100
24	W	51/56 (91%)	50 (98%)	1 (2%)	55	84
25	X	130/130 (100%)	123 (95%)	7 (5%)	22	53
26	Y	66/73 (90%)	62 (94%)	4 (6%)	18	48
27	Z	120/195 (62%)	113 (94%)	7 (6%)	20	50
28	1	56/56 (100%)	51 (91%)	5 (9%)	9	28
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	49	81
31	4	79/79 (100%)	76 (96%)	3 (4%)	33	67
All	All	3027/3441 (88%)	2884 (95%)	143 (5%)	26	59

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	W	43	PRO
25	X	122	ARG
27	Z	186	ARG
7	F	61	PHE
7	F	24	HIS

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	S	98	ASN
25	X	119	HIS
20	S	117	HIS
23	V	39	ASN
27	Z	133	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	237 (8%)	38 (1%)
2	B	121/122 (99%)	15 (12%)	3 (2%)
3	5	2/3 (66%)	1 (50%)	0
All	All	2870/3047 (94%)	253 (8%)	41 (1%)

5 of 253 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 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2011	A
1	A	2726	U
1	A	2313	C
1	A	2536	C
1	A	2791	U

## 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 237 ligands modelled in this entry, 234 are monoatomic - leaving 3 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	ACA	5	9078	37	7,7,8	1.26	1 (14%)	6,6,8	0.86	0
36	SPS	5	9080	32	20,23,23	1.94	6 (30%)	18,30,30	2.98	5 (27%)
37	PHA	5	9077	38,3	10,11,11	0.77	0	10,13,13	0.90	1 (10%)

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	ACA	5	9078	37	-	1/4/5/6	-
36	SPS	5	9080	32	-	5/15/18/18	0/1/1/1
37	PHA	5	9077	38,3	-	2/5/6/6	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	9080	SPS	C6-C1	4.34	1.54	1.43
36	5	9080	SPS	C16-S17	-3.47	1.76	1.79
36	5	9080	SPS	C9-C10	-3.19	1.41	1.48
36	5	9080	SPS	C1-N2	2.93	1.38	1.33
36	5	9080	SPS	C5-N4	2.92	1.38	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	9080	SPS	C6-C1-N2	-9.15	118.02	124.40
36	5	9080	SPS	C3-N2-C1	6.86	120.94	115.14
37	5	9077	PHA	CB-CA-C	-2.64	106.52	111.47
36	5	9080	SPS	O15-S15-C16	2.55	109.50	106.47
36	5	9080	SPS	C9-C10-N11	2.23	118.85	114.56

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	5	9080	SPS	C5-C6-C8-C9

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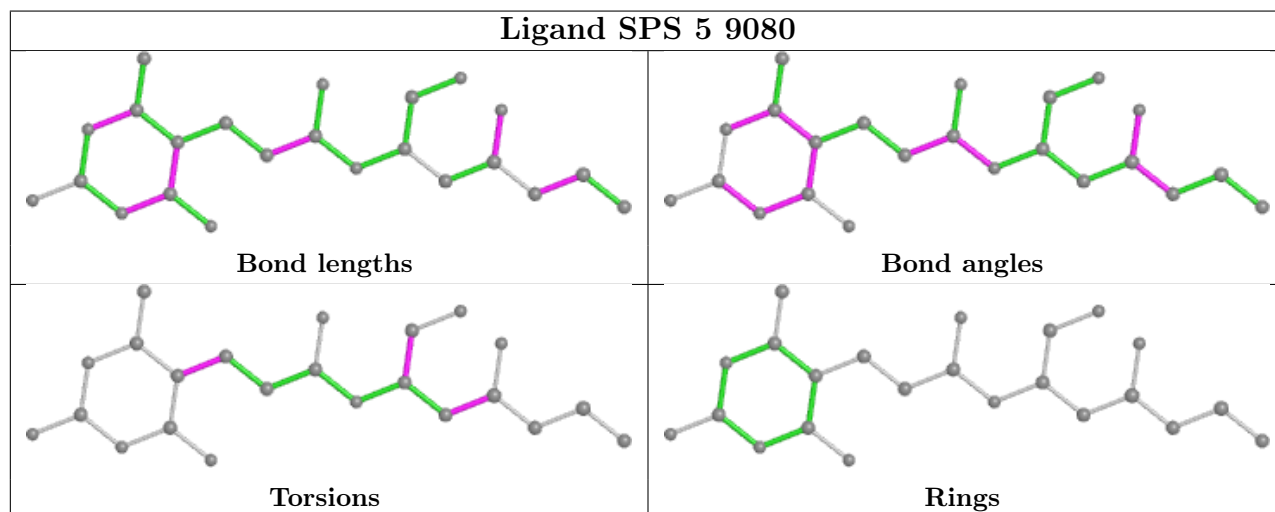
Mol	Chain	Res	Type	Atoms
36	5	9080	SPS	N11-C12-C13-O13
36	5	9080	SPS	C14-C12-C13-O13
36	5	9080	SPS	C12-C14-S15-O15
36	5	9080	SPS	C12-C14-S15-C16

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	9080	SPS	4	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

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, 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	A	2754/2922 (94%)	-0.03	73 (2%) 54 44	18, 43, 87, 135	0
2	B	122/122 (100%)	0.33	5 (4%) 37 27	35, 60, 87, 145	0
3	5	3/3 (100%)	-0.12	0 100 100	33, 33, 35, 36	0
4	C	237/239 (99%)	0.12	11 (4%) 32 22	24, 47, 79, 101	0
5	D	337/337 (100%)	-0.02	4 (1%) 79 73	25, 53, 79, 88	0
6	E	246/246 (100%)	-0.29	0 100 100	21, 42, 64, 75	0
7	F	140/176 (79%)	2.02	73 (52%) 0 0	51, 94, 112, 118	0
8	G	172/177 (97%)	0.92	16 (9%) 8 4	44, 67, 85, 92	0
9	H	119/119 (100%)	0.57	11 (9%) 9 5	45, 66, 91, 97	0
10	I	29/348 (8%)	2.37	18 (62%) 0 0	66, 85, 93, 96	0
11	J	156/167 (93%)	0.32	9 (5%) 23 15	34, 52, 77, 80	0
12	K	142/145 (97%)	-0.01	0 100 100	33, 49, 68, 86	0
13	L	132/132 (100%)	-0.11	2 (1%) 73 68	31, 50, 70, 80	0
14	M	145/164 (88%)	0.39	11 (7%) 13 7	20, 60, 98, 111	0
15	N	194/194 (100%)	-0.15	3 (1%) 73 68	28, 39, 58, 68	0
16	O	186/186 (100%)	0.53	20 (10%) 5 3	36, 59, 99, 111	0
17	P	115/115 (100%)	-0.06	1 (0%) 84 80	35, 49, 67, 77	0
18	Q	143/148 (96%)	0.11	1 (0%) 87 84	36, 52, 64, 74	0
19	R	95/95 (100%)	-0.12	1 (1%) 80 75	29, 40, 54, 70	0
20	S	150/154 (97%)	-0.24	0 100 100	29, 41, 61, 70	0
21	T	81/84 (96%)	0.08	2 (2%) 57 47	40, 54, 73, 80	0
22	U	119/119 (100%)	0.32	10 (8%) 11 5	36, 52, 76, 90	0
23	V	53/66 (80%)	0.19	1 (1%) 66 59	39, 53, 69, 77	0
24	W	65/70 (92%)	1.27	14 (21%) 0 0	49, 68, 105, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	154/154 (100%)	-0.26	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	32, 45, 63, 72	0
26	Y	82/91 (90%)	0.14	4 (4%) <span style="border: 1px solid red; padding: 2px;">29</span> <span style="border: 1px solid red; padding: 2px;">20</span>	40, 57, 79, 99	0
27	Z	142/240 (59%)	-0.10	2 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">70</span>	24, 41, 65, 82	0
28	1	73/73 (100%)	0.22	4 (5%) <span style="border: 1px solid red; padding: 2px;">25</span> <span style="border: 1px solid red; padding: 2px;">16</span>	46, 60, 71, 79	0
29	2	56/56 (100%)	-0.61	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	24, 29, 35, 43	0
30	3	46/48 (95%)	0.40	6 (13%) <span style="border: 1px solid red; padding: 2px;">3</span> <span style="border: 1px solid red; padding: 2px;">2</span>	31, 57, 84, 98	0
31	4	92/92 (100%)	0.08	1 (1%) <span style="border: 1px solid blue; padding: 2px;">80</span> <span style="border: 1px solid blue; padding: 2px;">75</span>	31, 51, 64, 78	0
All	All	6580/7282 (90%)	0.11	303 (4%) <span style="border: 1px solid red; padding: 2px;">32</span> <span style="border: 1px solid red; padding: 2px;">22</span>	18, 48, 88, 145	0

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	W	1	THR	10.6
2	B	3001	U	9.3
1	A	1172	G	6.7
1	A	1173	A	6.2
7	F	88	LEU	6.2

## 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, 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
33	NA	S	8386	1/1	0.37	0.92	91,91,91,91	0
33	NA	A	8384	1/1	0.38	0.81	75,75,75,75	0
32	MG	A	8024	1/1	0.48	1.23	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
39	CD	P	8405	1/1	0.56	0.14	174,174,174,174	0
33	NA	B	8351	1/1	0.59	0.53	78,78,78,78	0
33	NA	T	8312	1/1	0.67	0.65	79,79,79,79	0
33	NA	A	8385	1/1	0.68	0.41	50,50,50,50	0
33	NA	J	8322	1/1	0.70	0.31	61,61,61,61	0
33	NA	A	8307	1/1	0.70	0.27	46,46,46,46	0
33	NA	A	8324	1/1	0.71	0.17	55,55,55,55	0
32	MG	B	8095	1/1	0.71	0.18	70,70,70,70	0
33	NA	A	8368	1/1	0.73	0.20	56,56,56,56	0
32	MG	A	8113	1/1	0.74	0.20	43,43,43,43	0
33	NA	A	8329	1/1	0.75	0.23	54,54,54,54	0
33	NA	A	8311	1/1	0.76	0.29	55,55,55,55	0
33	NA	A	8352	1/1	0.76	0.41	71,71,71,71	0
38	ACA	5	9078	8/9	0.79	0.38	45,53,55,55	0
33	NA	A	8333	1/1	0.79	0.15	33,33,33,33	0
33	NA	B	8383	1/1	0.80	0.61	69,69,69,69	0
32	MG	A	8076	1/1	0.80	0.09	50,50,50,50	0
35	CL	O	8507	1/1	0.84	0.27	59,59,59,59	0
33	NA	A	8359	1/1	0.84	0.38	40,40,40,40	0
33	NA	A	8364	1/1	0.84	0.27	39,39,39,39	0
33	NA	A	8363	1/1	0.85	0.25	49,49,49,49	0
33	NA	A	8371	1/1	0.85	0.31	61,61,61,61	0
33	NA	A	8372	1/1	0.86	0.44	58,58,58,58	0
35	CL	K	8502	1/1	0.87	0.14	66,66,66,66	0
33	NA	A	8313	1/1	0.88	0.10	62,62,62,62	0
33	NA	A	8326	1/1	0.88	0.33	37,37,37,37	0
33	NA	M	8380	1/1	0.89	0.41	64,64,64,64	0
33	NA	A	8382	1/1	0.89	0.17	72,72,72,72	0
32	MG	A	8089	1/1	0.89	0.08	58,58,58,58	0
33	NA	A	8314	1/1	0.89	0.19	38,38,38,38	0
33	NA	A	8310	1/1	0.89	0.26	39,39,39,39	0
33	NA	A	8357	1/1	0.89	0.08	53,53,53,53	0
32	MG	1	8105	1/1	0.89	0.28	32,32,32,32	0
33	NA	E	8304	1/1	0.90	0.17	33,33,33,33	0
33	NA	A	8308	1/1	0.90	0.10	43,43,43,43	0
32	MG	A	8082	1/1	0.90	0.12	53,53,53,53	0
32	MG	A	8045	1/1	0.91	0.09	56,56,56,56	0
33	NA	A	8369	1/1	0.91	0.14	49,49,49,49	0
34	K	A	8390	1/1	0.91	0.36	70,70,70,70	0
32	MG	A	8090	1/1	0.91	0.28	70,70,70,70	0
32	MG	A	8101	1/1	0.91	0.13	52,52,52,52	0
32	MG	A	8087	1/1	0.91	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8341	1/1	0.91	0.13	41,41,41,41	0
32	MG	A	8114	1/1	0.92	0.22	54,54,54,54	0
33	NA	A	8362	1/1	0.92	0.31	64,64,64,64	0
33	NA	A	8375	1/1	0.92	0.59	47,47,47,47	0
32	MG	A	8085	1/1	0.92	0.11	45,45,45,45	0
32	MG	A	8106	1/1	0.92	0.08	52,52,52,52	0
33	NA	A	8365	1/1	0.92	0.23	43,43,43,43	0
33	NA	A	8366	1/1	0.92	0.49	68,68,68,68	0
33	NA	A	8355	1/1	0.92	0.55	56,56,56,56	0
32	MG	A	8049	1/1	0.92	0.62	77,77,77,77	0
32	MG	A	8057	1/1	0.93	0.13	40,40,40,40	0
33	NA	A	8335	1/1	0.93	0.22	43,43,43,43	0
33	NA	A	8373	1/1	0.93	0.48	50,50,50,50	0
33	NA	N	8347	1/1	0.93	0.12	23,23,23,23	0
33	NA	A	8301	1/1	0.93	0.17	46,46,46,46	0
33	NA	A	8377	1/1	0.93	0.22	66,66,66,66	0
33	NA	U	8343	1/1	0.93	0.15	33,33,33,33	0
33	NA	A	8342	1/1	0.93	0.22	40,40,40,40	0
35	CL	A	8517	1/1	0.93	0.14	59,59,59,59	0
33	NA	A	8303	1/1	0.93	0.18	43,43,43,43	0
35	CL	K	8521	1/1	0.93	0.10	50,50,50,50	0
33	NA	A	8353	1/1	0.93	0.15	23,23,23,23	0
35	CL	Z	8520	1/1	0.93	0.12	42,42,42,42	0
32	MG	A	8050	1/1	0.93	0.15	64,64,64,64	0
33	NA	A	8332	1/1	0.93	0.14	29,29,29,29	0
32	MG	A	8111	1/1	0.94	0.10	51,51,51,51	0
32	MG	A	8047	1/1	0.94	0.15	66,66,66,66	0
32	MG	A	8066	1/1	0.94	0.23	84,84,84,84	0
33	NA	A	8319	1/1	0.94	0.10	36,36,36,36	0
32	MG	A	8070	1/1	0.94	0.15	47,47,47,47	0
32	MG	A	8027	1/1	0.94	0.08	49,49,49,49	0
35	CL	A	8511	1/1	0.94	0.11	48,48,48,48	0
32	MG	A	8094	1/1	0.94	0.04	63,63,63,63	0
35	CL	C	8509	1/1	0.94	0.19	56,56,56,56	0
32	MG	A	8046	1/1	0.94	0.08	47,47,47,47	0
33	NA	A	8305	1/1	0.94	0.13	35,35,35,35	0
32	MG	A	8103	1/1	0.94	0.18	61,61,61,61	0
33	NA	C	8345	1/1	0.94	0.13	44,44,44,44	0
35	CL	4	8504	1/1	0.94	0.14	67,67,67,67	0
32	MG	A	8083	1/1	0.94	0.09	41,41,41,41	0
32	MG	A	8108	1/1	0.94	0.13	60,60,60,60	0
32	MG	A	8063	1/1	0.95	0.05	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8032	1/1	0.95	0.08	28,28,28,28	0
33	NA	A	8306	1/1	0.95	0.52	32,32,32,32	0
32	MG	A	8053	1/1	0.95	0.14	50,50,50,50	0
33	NA	S	8337	1/1	0.95	0.19	28,28,28,28	0
33	NA	A	8367	1/1	0.95	0.10	44,44,44,44	0
32	MG	A	8099	1/1	0.95	0.12	48,48,48,48	0
33	NA	A	8340	1/1	0.95	0.47	44,44,44,44	0
33	NA	A	8309	1/1	0.95	0.09	32,32,32,32	0
35	CL	A	8503	1/1	0.95	0.13	46,46,46,46	0
32	MG	A	8100	1/1	0.95	0.16	65,65,65,65	0
32	MG	A	8119	1/1	0.95	0.14	41,41,41,41	0
32	MG	A	8041	1/1	0.95	0.16	53,53,53,53	0
32	MG	U	8073	1/1	0.95	0.09	46,46,46,46	0
33	NA	A	8356	1/1	0.95	0.28	47,47,47,47	0
33	NA	A	8317	1/1	0.95	0.17	45,45,45,45	0
33	NA	A	8358	1/1	0.95	0.80	82,82,82,82	0
32	MG	A	8088	1/1	0.95	0.09	30,30,30,30	0
33	NA	A	8360	1/1	0.95	0.56	39,39,39,39	0
32	MG	A	8104	1/1	0.95	0.26	52,52,52,52	0
33	NA	A	8334	1/1	0.96	0.06	32,32,32,32	0
32	MG	L	8069	1/1	0.96	0.07	50,50,50,50	0
33	NA	A	8378	1/1	0.96	0.54	47,47,47,47	0
33	NA	A	8336	1/1	0.96	0.06	53,53,53,53	0
33	NA	A	8338	1/1	0.96	0.09	41,41,41,41	0
32	MG	A	8062	1/1	0.96	0.10	48,48,48,48	0
32	MG	A	8091	1/1	0.96	0.05	69,69,69,69	0
32	MG	A	8092	1/1	0.96	0.13	79,79,79,79	0
33	NA	A	8350	1/1	0.96	0.24	32,32,32,32	0
32	MG	A	8004	1/1	0.96	0.07	26,26,26,26	0
32	MG	A	8096	1/1	0.96	0.07	46,46,46,46	0
33	NA	K	8346	1/1	0.96	0.08	40,40,40,40	0
33	NA	A	8354	1/1	0.96	0.27	34,34,34,34	0
32	MG	A	8098	1/1	0.96	0.13	36,36,36,36	0
32	MG	A	8042	1/1	0.96	0.13	31,31,31,31	0
32	MG	A	8068	1/1	0.96	0.16	50,50,50,50	0
32	MG	A	8044	1/1	0.96	0.06	36,36,36,36	0
32	MG	A	8075	1/1	0.96	0.07	37,37,37,37	0
32	MG	A	8051	1/1	0.96	0.08	57,57,57,57	0
32	MG	A	8079	1/1	0.96	0.11	27,27,27,27	0
32	MG	A	8107	1/1	0.96	0.05	43,43,43,43	0
35	CL	A	8515	1/1	0.96	0.34	65,65,65,65	0
32	MG	A	8005	1/1	0.96	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8054	1/1	0.96	0.10	24,24,24,24	0
35	CL	K	8501	1/1	0.96	0.12	55,55,55,55	0
32	MG	A	8055	1/1	0.96	0.08	43,43,43,43	0
32	MG	A	8007	1/1	0.96	0.06	16,16,16,16	0
33	NA	A	8328	1/1	0.96	0.32	34,34,34,34	0
35	CL	P	8508	1/1	0.96	0.10	62,62,62,62	0
32	MG	A	8116	1/1	0.96	0.11	51,51,51,51	0
33	NA	A	8331	1/1	0.96	0.17	31,31,31,31	0
36	SPS	5	9080	23/23	0.96	0.21	30,33,47,49	0
37	PHA	5	9077	11/11	0.96	0.24	41,45,52,53	0
32	MG	A	8059	1/1	0.96	0.13	35,35,35,35	0
32	MG	A	8061	1/1	0.96	0.07	34,34,34,34	0
33	NA	A	8318	1/1	0.97	0.41	55,55,55,55	0
32	MG	A	8071	1/1	0.97	0.04	63,63,63,63	0
33	NA	A	8321	1/1	0.97	0.19	54,54,54,54	0
32	MG	5	8118	1/1	0.97	0.12	29,29,29,29	0
32	MG	A	8016	1/1	0.97	0.11	39,39,39,39	0
33	NA	A	8361	1/1	0.97	0.28	47,47,47,47	0
33	NA	R	8348	1/1	0.97	0.17	42,42,42,42	0
32	MG	A	8056	1/1	0.97	0.06	39,39,39,39	0
32	MG	Z	8109	1/1	0.97	0.07	33,33,33,33	0
32	MG	A	8033	1/1	0.97	0.10	28,28,28,28	0
32	MG	A	8081	1/1	0.97	0.12	43,43,43,43	0
33	NA	A	8302	1/1	0.97	0.14	46,46,46,46	0
32	MG	A	8058	1/1	0.97	0.11	37,37,37,37	0
35	CL	A	8505	1/1	0.97	0.16	49,49,49,49	0
32	MG	A	8037	1/1	0.97	0.05	34,34,34,34	0
35	CL	A	8512	1/1	0.97	0.09	47,47,47,47	0
35	CL	A	8514	1/1	0.97	0.12	46,46,46,46	0
32	MG	A	8040	1/1	0.97	0.12	53,53,53,53	0
35	CL	A	8516	1/1	0.97	0.13	56,56,56,56	0
33	NA	A	8370	1/1	0.97	0.41	57,57,57,57	0
32	MG	A	8022	1/1	0.97	0.12	40,40,40,40	0
33	NA	A	8339	1/1	0.97	0.14	22,22,22,22	0
32	MG	A	8008	1/1	0.97	0.05	35,35,35,35	0
32	MG	A	8064	1/1	0.97	0.14	31,31,31,31	0
32	MG	A	8052	1/1	0.97	0.06	40,40,40,40	0
33	NA	A	8349	1/1	0.97	0.14	41,41,41,41	0
33	NA	A	8379	1/1	0.97	0.12	45,45,45,45	0
32	MG	A	8067	1/1	0.97	0.12	43,43,43,43	0
32	MG	A	8043	1/1	0.97	0.08	39,39,39,39	0
32	MG	A	8117	1/1	0.97	0.08	25,25,25,25	0

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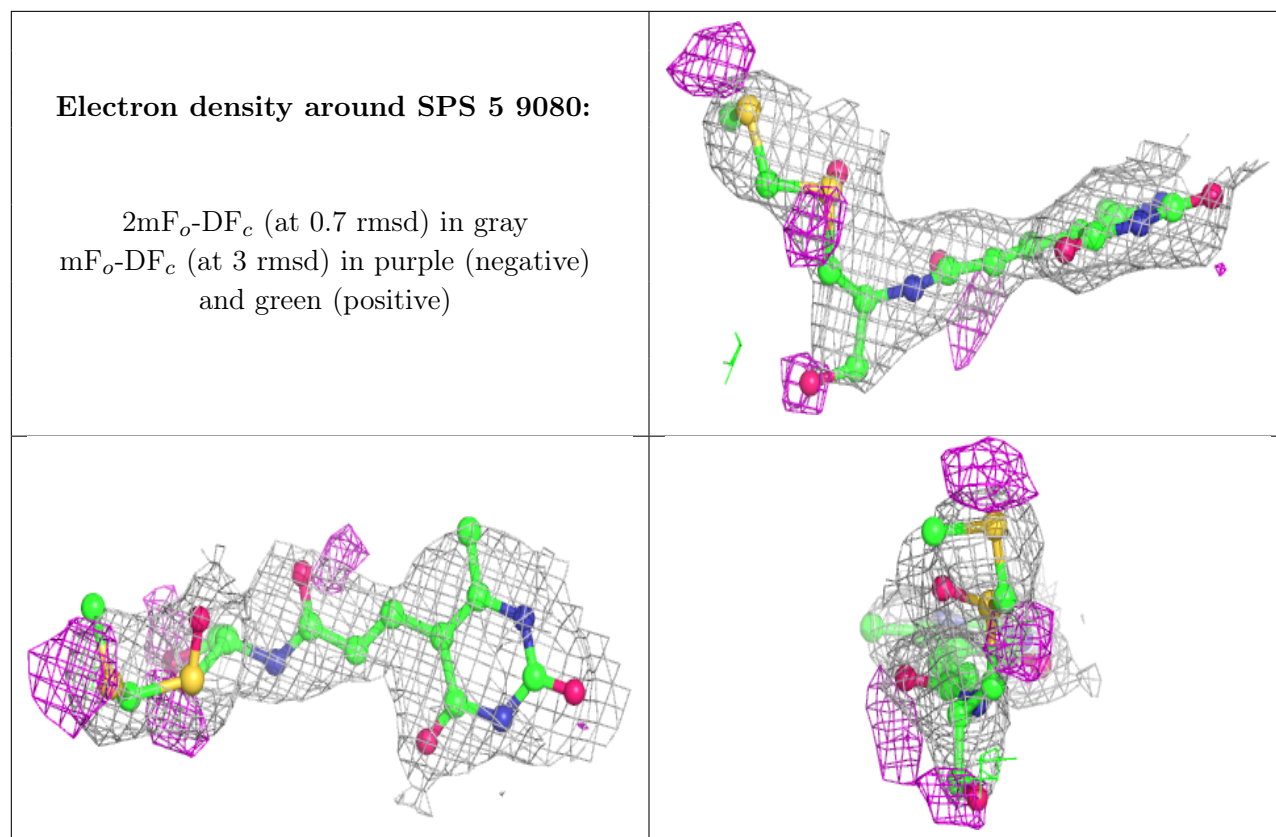
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8316	1/1	0.97	0.20	40,40,40,40	0
32	MG	A	8013	1/1	0.97	0.17	32,32,32,32	0
32	MG	A	8035	1/1	0.98	0.03	52,52,52,52	0
32	MG	A	8036	1/1	0.98	0.05	32,32,32,32	0
32	MG	A	8021	1/1	0.98	0.11	33,33,33,33	0
32	MG	A	8038	1/1	0.98	0.09	27,27,27,27	0
32	MG	A	8110	1/1	0.98	0.11	35,35,35,35	0
32	MG	A	8011	1/1	0.98	0.09	26,26,26,26	0
32	MG	A	8112	1/1	0.98	0.17	28,28,28,28	0
32	MG	A	8023	1/1	0.98	0.06	39,39,39,39	0
32	MG	A	8001	1/1	0.98	0.07	27,27,27,27	0
32	MG	A	8115	1/1	0.98	0.06	42,42,42,42	0
33	NA	A	8374	1/1	0.98	0.67	53,53,53,53	0
35	CL	A	8513	1/1	0.98	0.11	50,50,50,50	0
32	MG	A	8093	1/1	0.98	0.08	49,49,49,49	0
33	NA	A	8376	1/1	0.98	0.14	47,47,47,47	0
32	MG	A	8072	1/1	0.98	0.10	56,56,56,56	0
32	MG	A	8025	1/1	0.98	0.07	40,40,40,40	0
35	CL	A	8522	1/1	0.98	0.16	55,55,55,55	0
32	MG	A	8097	1/1	0.98	0.17	28,28,28,28	0
35	CL	D	8519	1/1	0.98	0.11	40,40,40,40	0
33	NA	A	8381	1/1	0.98	0.23	44,44,44,44	0
32	MG	A	8015	1/1	0.98	0.09	29,29,29,29	0
33	NA	A	8320	1/1	0.98	0.11	38,38,38,38	0
35	CL	M	8510	1/1	0.98	0.16	47,47,47,47	0
35	CL	N	8518	1/1	0.98	0.12	39,39,39,39	0
32	MG	A	8029	1/1	0.98	0.08	41,41,41,41	0
32	MG	A	8006	1/1	0.98	0.04	30,30,30,30	0
35	CL	S	8506	1/1	0.98	0.11	46,46,46,46	0
32	MG	A	8019	1/1	0.98	0.04	29,29,29,29	0
33	NA	A	8327	1/1	0.98	0.12	41,41,41,41	0
32	MG	A	8102	1/1	0.98	0.12	45,45,45,45	0
32	MG	4	8078	1/1	0.98	0.04	41,41,41,41	0
33	NA	A	8330	1/1	0.98	0.22	34,34,34,34	0
32	MG	A	8048	1/1	0.98	0.16	58,58,58,58	0
32	MG	A	8018	1/1	0.99	0.09	31,31,31,31	0
32	MG	C	8065	1/1	0.99	0.11	31,31,31,31	0
32	MG	A	8077	1/1	0.99	0.06	27,27,27,27	0
32	MG	A	8030	1/1	0.99	0.10	32,32,32,32	0
32	MG	A	8080	1/1	0.99	0.05	36,36,36,36	0
33	NA	A	8325	1/1	0.99	0.36	50,50,50,50	0
32	MG	A	8031	1/1	0.99	0.05	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8060	1/1	0.99	0.18	42,42,42,42	0
32	MG	A	8003	1/1	0.99	0.12	26,26,26,26	0
32	MG	A	8084	1/1	0.99	0.05	40,40,40,40	0
32	MG	A	8012	1/1	0.99	0.09	28,28,28,28	0
32	MG	A	8086	1/1	0.99	0.17	45,45,45,45	0
32	MG	A	8034	1/1	0.99	0.07	33,33,33,33	0
32	MG	A	8002	1/1	0.99	0.06	28,28,28,28	0
32	MG	A	8014	1/1	0.99	0.06	25,25,25,25	0
32	MG	A	8009	1/1	0.99	0.04	26,26,26,26	0
32	MG	A	8010	1/1	0.99	0.09	35,35,35,35	0
32	MG	A	8039	1/1	0.99	0.08	42,42,42,42	0
32	MG	A	8026	1/1	0.99	0.07	26,26,26,26	0
32	MG	A	8017	1/1	0.99	0.03	19,19,19,19	0
33	NA	A	8315	1/1	0.99	0.10	32,32,32,32	0
32	MG	A	8074	1/1	0.99	0.03	29,29,29,29	0
33	NA	A	8344	1/1	0.99	0.05	25,25,25,25	0
34	K	A	8391	1/1	0.99	0.25	48,48,48,48	0
32	MG	A	8028	1/1	0.99	0.09	34,34,34,34	0
39	CD	1	8403	1/1	0.99	0.08	62,62,62,62	0
39	CD	2	8402	1/1	0.99	0.07	56,56,56,56	0
39	CD	4	8404	1/1	0.99	0.06	57,57,57,57	0
32	MG	A	8020	1/1	1.00	0.07	28,28,28,28	0
33	NA	A	8323	1/1	1.00	0.10	42,42,42,42	0
39	CD	V	8401	1/1	1.00	0.07	62,62,62,62	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.