



# wwPDB X-ray Structure Validation Summary Report

Aug 22, 2023 – 04:46 PM EDT

PDB ID : 3CJT  
Title : Ribosomal protein L11 methyltransferase (PrmA) in complex with dimethylated ribosomal protein L11  
Authors : Demirci, H.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2008-03-13  
Resolution : 2.30 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 : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

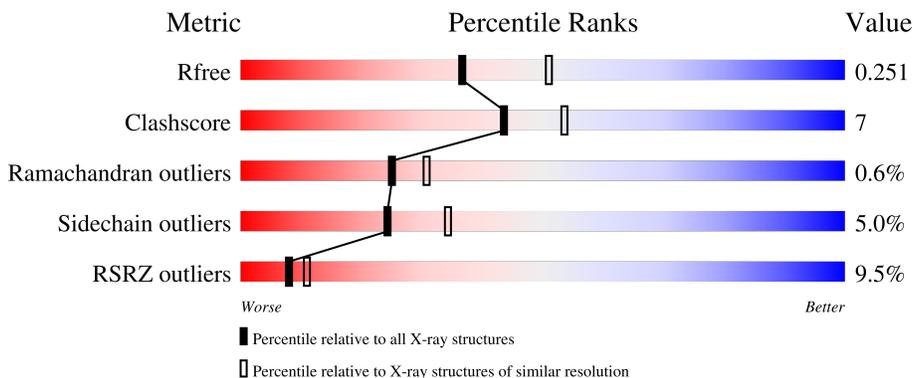
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	254	
1	C	254	
1	E	254	
1	G	254	
1	I	254	

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Mol	Chain	Length	Quality of chain
1	K	254	
1	M	254	
1	O	254	
2	B	147	
2	D	147	
2	F	147	
2	H	147	
2	J	147	
2	L	147	
2	N	147	
2	P	147	

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
4	CL	I	258	-	-	X	-
7	2MM	M	257	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 23555 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 protein called Ribosomal protein L11 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	Total 1966	C 1278	N 338	O 346	S 4	0	2	0
1	C	250	Total 1922	C 1245	N 333	O 341	S 3	5	0	0
1	E	254	Total 1953	C 1267	N 337	O 345	S 4	0	0	0
1	G	251	Total 1926	C 1247	N 334	O 342	S 3	5	0	0
1	I	254	Total 1961	C 1273	N 338	O 346	S 4	0	1	0
1	K	250	Total 1922	C 1245	N 333	O 341	S 3	5	0	0
1	M	254	Total 1961	C 1273	N 338	O 346	S 4	0	1	0
1	O	250	Total 1922	C 1245	N 333	O 341	S 3	5	0	0

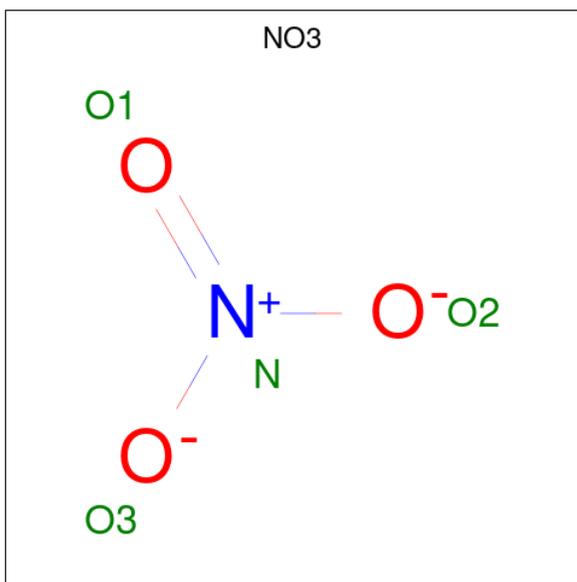
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	ALA	HIS	engineered mutation	UNP Q84BQ9
C	104	ALA	HIS	engineered mutation	UNP Q84BQ9
E	104	ALA	HIS	engineered mutation	UNP Q84BQ9
G	104	ALA	HIS	engineered mutation	UNP Q84BQ9
I	104	ALA	HIS	engineered mutation	UNP Q84BQ9
K	104	ALA	HIS	engineered mutation	UNP Q84BQ9
M	104	ALA	HIS	engineered mutation	UNP Q84BQ9
O	104	ALA	HIS	engineered mutation	UNP Q84BQ9

- Molecule 2 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			921	588	166	162	5			
2	D	72	Total	C	N	O	S	4	0	0
			525	341	88	93	3			
2	F	130	Total	C	N	O	S	0	0	0
			950	607	170	168	5			
2	H	71	Total	C	N	O	S	4	0	0
			520	338	87	92	3			
2	J	127	Total	C	N	O	S	0	0	0
			922	588	166	163	5			
2	L	72	Total	C	N	O	S	4	0	0
			525	341	88	93	3			
2	N	130	Total	C	N	O	S	0	0	0
			946	604	169	168	5			
2	P	72	Total	C	N	O	S	4	0	0
			525	341	88	93	3			

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	N O	0	0
			4	1 3		
3	B	1	Total	N O	0	0
			4	1 3		
3	E	1	Total	N O	0	0
			4	1 3		
3	F	1	Total	N O	0	0
			4	1 3		

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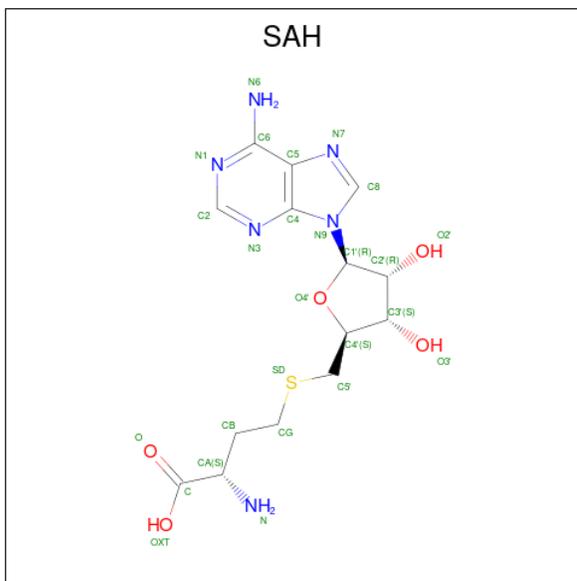
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	N	O	0	0
			4	1	3		
3	I	1	Total	N	O	0	0
			4	1	3		
3	M	1	Total	N	O	0	0
			4	1	3		
3	N	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	I	2	Total	Cl	0	0
			2	2		

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



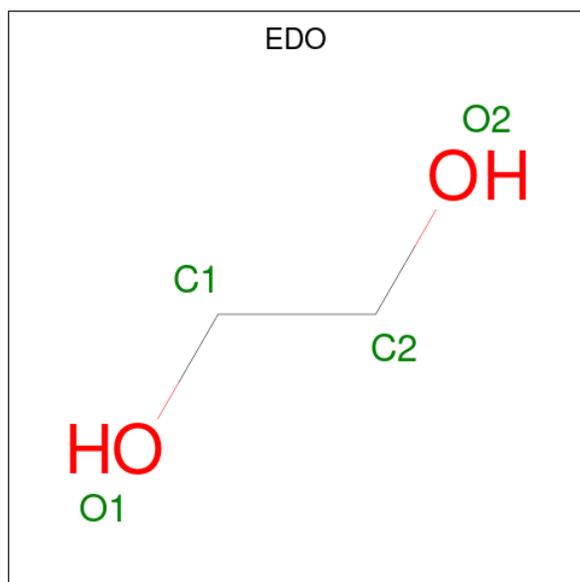
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	I	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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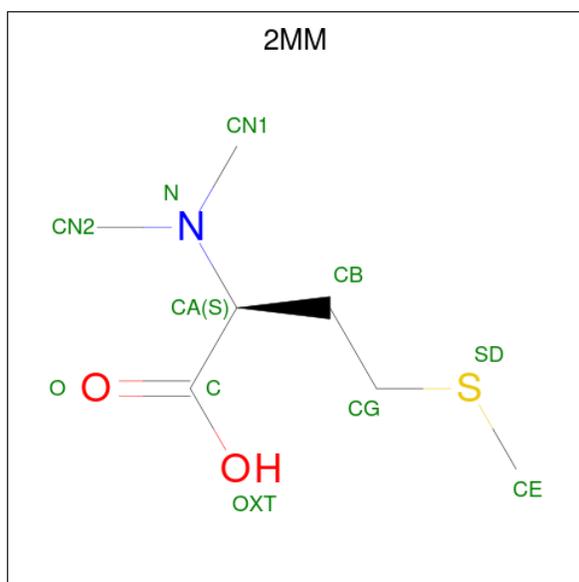
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	M	1	26	14	6	5	1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



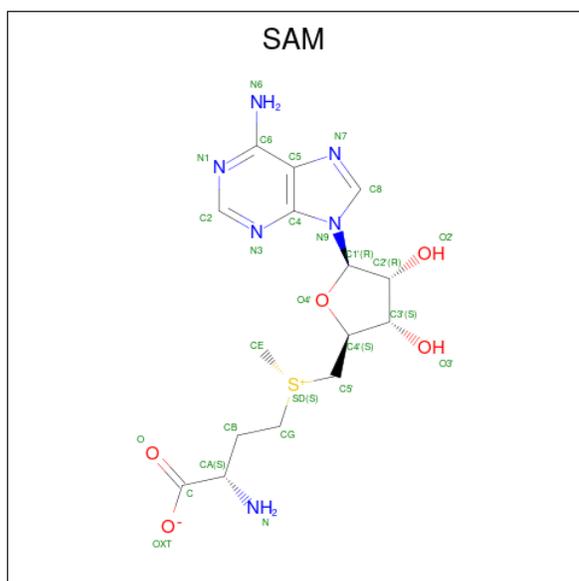
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
6	B	1	4	2	2	0	0

- Molecule 7 is N,N-dimethyl-L-methionine (three-letter code: 2MM) (formula:  $C_7H_{15}NO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
7	B	1	Total	10	7	1	1	1	0	0
7	F	1	Total	10	7	1	1	1	0	0
7	J	1	Total	10	7	1	1	1	0	0
7	M	1	Total	10	7	1	1	1	0	0

- Molecule 8 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula:  $C_{15}H_{22}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
8	G	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
8	K	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
8	O	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

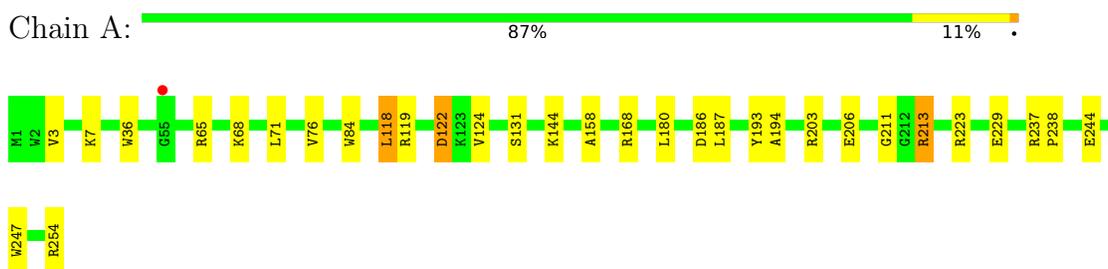
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	263	Total	O	0	5
			268	268		
9	B	87	Total	O	0	2
			89	89		
9	C	173	Total	O	0	0
			173	173		
9	D	25	Total	O	0	0
			25	25		
9	E	248	Total	O	0	0
			248	248		
9	F	61	Total	O	0	0
			61	61		
9	G	198	Total	O	0	0
			198	198		
9	H	22	Total	O	0	0
			22	22		
9	I	200	Total	O	0	0
			200	200		
9	J	67	Total	O	0	0
			67	67		
9	K	142	Total	O	0	0
			142	142		
9	L	10	Total	O	0	0
			10	10		
9	M	193	Total	O	0	0
			193	193		
9	N	46	Total	O	0	0
			46	46		
9	O	145	Total	O	0	0
			145	145		
9	P	5	Total	O	0	0
			5	5		

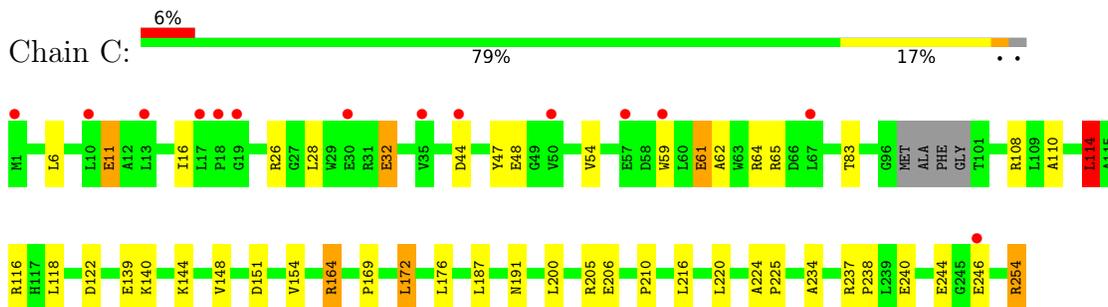
### 3 Residue-property plots [i](#)

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.

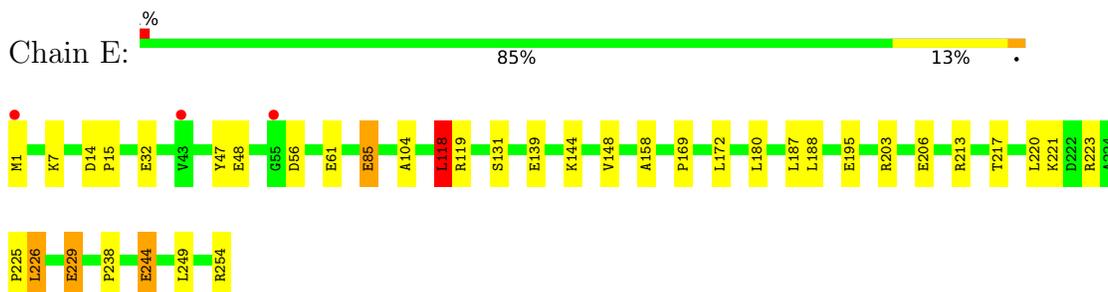
- Molecule 1: Ribosomal protein L11 methyltransferase



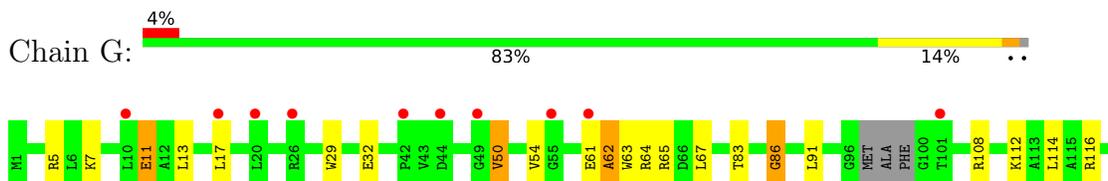
- Molecule 1: Ribosomal protein L11 methyltransferase



- Molecule 1: Ribosomal protein L11 methyltransferase



- Molecule 1: Ribosomal protein L11 methyltransferase

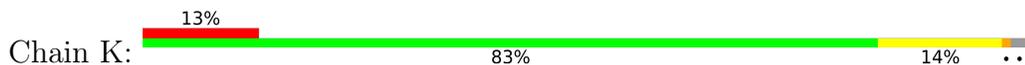




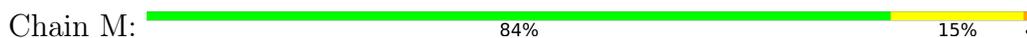
- Molecule 1: Ribosomal protein L11 methyltransferase



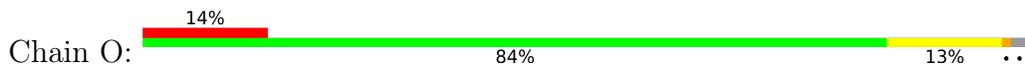
- Molecule 1: Ribosomal protein L11 methyltransferase



- Molecule 1: Ribosomal protein L11 methyltransferase



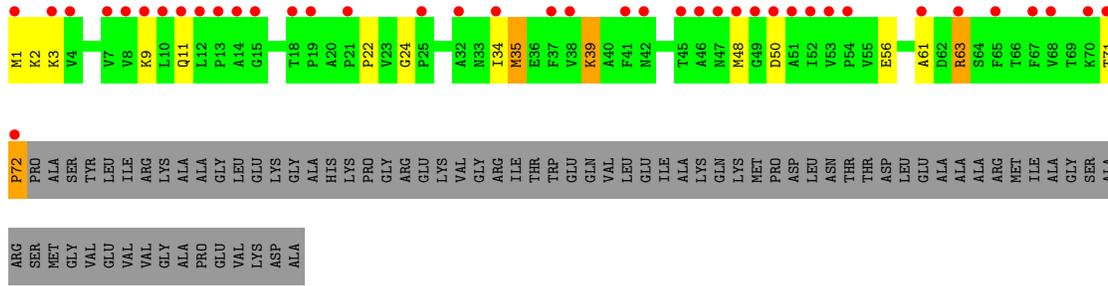
- Molecule 1: Ribosomal protein L11 methyltransferase



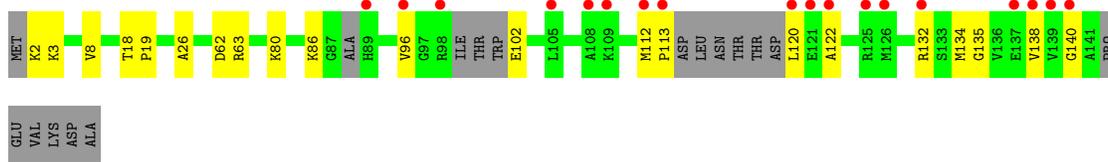
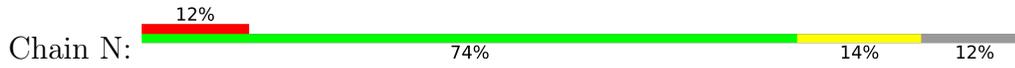
- Molecule 2: 50S ribosomal protein L11



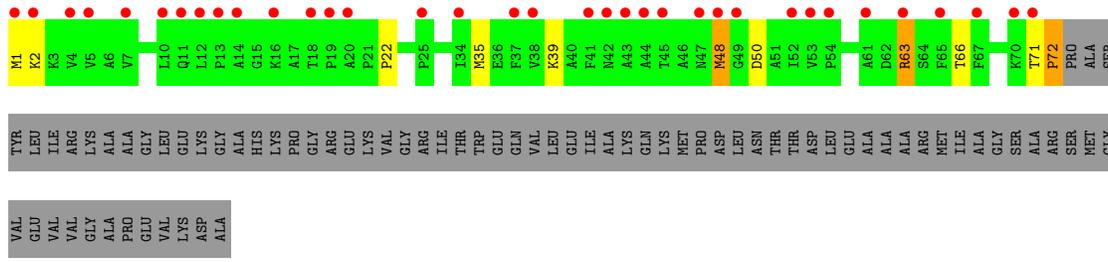
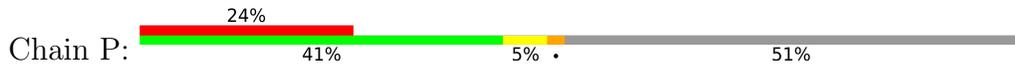




• Molecule 2: 50S ribosomal protein L11



• Molecule 2: 50S ribosomal protein L11



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.82Å 69.94Å 379.01Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	29.74 – 2.30 29.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.74-2.30) 94.1 (29.73-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194 , 0.259 0.190 , 0.251	Depositor DCC
$R_{free}$ test set	7909 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 31.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.407 for -k,-h,-l 0.410 for k,h,-l 0.387 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23555	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: 2MM, CL, SAH, NO3, EDO, SAM

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	0.67	1/2025 (0.0%)	0.73	4/2761 (0.1%)
1	C	2.15	4/1976 (0.2%)	0.84	5/2694 (0.2%)
1	E	0.67	2/2009 (0.1%)	0.74	1/2739 (0.0%)
1	G	2.25	3/1980 (0.2%)	0.86	4/2699 (0.1%)
1	I	0.59	0/2017	0.70	1/2750 (0.0%)
1	K	2.08	4/1976 (0.2%)	0.77	3/2694 (0.1%)
1	M	0.60	0/2017	0.70	2/2750 (0.1%)
1	O	1.67	4/1976 (0.2%)	0.77	5/2694 (0.2%)
2	B	2.00	2/936 (0.2%)	0.84	1/1261 (0.1%)
2	D	1.56	2/536 (0.4%)	1.31	5/730 (0.7%)
2	F	0.62	2/964 (0.2%)	0.70	0/1298
2	H	0.86	2/531 (0.4%)	2.78	4/723 (0.6%)
2	J	0.54	0/937	0.67	0/1264
2	L	1.52	3/536 (0.6%)	1.14	4/730 (0.5%)
2	N	0.53	1/960 (0.1%)	0.62	0/1294
2	P	0.96	2/536 (0.4%)	1.17	5/730 (0.7%)
All	All	1.43	32/21912 (0.1%)	0.90	44/29811 (0.1%)

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	C	0	1
1	G	0	1
2	D	0	1
2	H	0	1
2	L	0	1
2	P	0	1
All	All	0	6

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	11	GLU	CD-OE1	77.43	2.10	1.25
1	C	11	GLU	CD-OE1	71.32	2.04	1.25
1	K	11	GLU	CG-CD	62.97	2.46	1.51
2	B	140	GLY	C-O	58.07	2.16	1.23
1	G	11	GLU	CD-OE2	56.12	1.87	1.25

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	63	ARG	NE-CZ-NH2	-68.41	86.10	120.30
2	D	63	ARG	NE-CZ-NH2	-26.56	107.02	120.30
2	P	63	ARG	NE-CZ-NH2	-22.95	108.82	120.30
2	H	63	ARG	NH1-CZ-NH2	22.45	144.10	119.40
2	L	63	ARG	NH1-CZ-NH2	-22.45	94.70	119.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	11	GLU	Sidechain
2	D	63	ARG	Sidechain
1	G	11	GLU	Sidechain
2	H	63	ARG	Sidechain
2	L	63	ARG	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1966	0	1974	27	0
1	C	1922	0	1917	34	0
1	E	1953	0	1953	27	0
1	G	1926	0	1920	24	0
1	I	1961	0	1963	22	0
1	K	1922	0	1917	30	0
1	M	1961	0	1963	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1922	0	1917	22	0
2	B	921	0	974	13	1
2	D	525	0	549	8	0
2	F	950	0	1001	22	0
2	H	520	0	548	7	0
2	J	922	0	968	14	0
2	L	525	0	549	9	0
2	N	946	0	990	16	0
2	P	525	0	549	5	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	1	0
3	I	8	0	0	0	0
3	M	4	0	0	0	0
3	N	4	0	0	0	0
4	A	2	0	0	0	0
4	I	2	0	0	2	0
5	A	26	0	19	0	0
5	E	26	0	19	0	0
5	I	26	0	19	0	0
5	M	26	0	19	0	0
6	A	4	0	6	1	0
6	B	4	0	6	0	0
7	B	10	0	14	2	0
7	F	10	0	14	4	0
7	J	10	0	14	1	0
7	M	10	0	14	9	0
8	C	27	0	22	3	0
8	G	27	0	22	2	0
8	K	27	0	22	4	0
8	O	27	0	22	5	0
9	A	268	0	0	7	0
9	B	89	0	0	0	0
9	C	173	0	0	7	0
9	D	25	0	0	1	0
9	E	248	0	0	5	0
9	F	61	0	0	3	0
9	G	198	0	0	6	1
9	H	22	0	0	1	0
9	I	200	0	0	7	0
9	J	67	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	142	0	0	8	0
9	L	10	0	0	1	0
9	M	193	0	0	5	0
9	N	46	0	0	0	0
9	O	145	0	0	2	0
9	P	5	0	0	0	0
All	All	23555	0	21884	290	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 7.

The worst 5 of 290 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:GLU:HG3	9:E:297:HOH:O	1.33	1.26
7:M:257:2MM:O	2:N:2:LYS:N	1.78	1.17
1:O:61:GLU:HG3	1:O:65:ARG:HB3	1.38	1.04
1:C:164:ARG:HG2	1:C:164:ARG:HH11	1.25	1.01
2:L:1:MET:H3	2:L:2:LYS:HA	1.31	0.95

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)
2:B:134:MET:O	9:G:459:HOH:O[2_555]	2.15	0.05

## 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
1	A	254/254 (100%)	243 (96%)	11 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	246/254 (97%)	237 (96%)	8 (3%)	1 (0%)	34	42
1	E	252/254 (99%)	247 (98%)	4 (2%)	1 (0%)	34	42
1	G	247/254 (97%)	238 (96%)	6 (2%)	3 (1%)	13	14
1	I	253/254 (100%)	242 (96%)	11 (4%)	0	100	100
1	K	246/254 (97%)	236 (96%)	8 (3%)	2 (1%)	19	23
1	M	253/254 (100%)	246 (97%)	7 (3%)	0	100	100
1	O	246/254 (97%)	236 (96%)	8 (3%)	2 (1%)	19	23
2	B	120/147 (82%)	112 (93%)	7 (6%)	1 (1%)	19	23
2	D	70/147 (48%)	64 (91%)	4 (6%)	2 (3%)	4	3
2	F	122/147 (83%)	113 (93%)	7 (6%)	2 (2%)	9	9
2	H	69/147 (47%)	65 (94%)	3 (4%)	1 (1%)	11	11
2	J	121/147 (82%)	115 (95%)	6 (5%)	0	100	100
2	L	70/147 (48%)	66 (94%)	4 (6%)	0	100	100
2	N	122/147 (83%)	120 (98%)	1 (1%)	1 (1%)	19	23
2	P	70/147 (48%)	66 (94%)	3 (4%)	1 (1%)	11	11
All	All	2761/3208 (86%)	2646 (96%)	98 (4%)	17 (1%)	25	31

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	50	ASP
1	E	32	GLU
2	F	124	ALA
1	G	62	ALA
1	G	86	GLY

### 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	
1	A	190/188 (101%)	186 (98%)	4 (2%)	53	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	185/188 (98%)	172 (93%)	13 (7%)	15	19
1	E	188/188 (100%)	181 (96%)	7 (4%)	34	48
1	G	185/188 (98%)	171 (92%)	14 (8%)	13	16
1	I	189/188 (100%)	181 (96%)	8 (4%)	30	42
1	K	185/188 (98%)	179 (97%)	6 (3%)	39	54
1	M	189/188 (100%)	178 (94%)	11 (6%)	20	27
1	O	185/188 (98%)	172 (93%)	13 (7%)	15	19
2	B	92/111 (83%)	89 (97%)	3 (3%)	38	53
2	D	54/111 (49%)	52 (96%)	2 (4%)	34	48
2	F	95/111 (86%)	86 (90%)	9 (10%)	8	10
2	H	54/111 (49%)	52 (96%)	2 (4%)	34	48
2	J	91/111 (82%)	88 (97%)	3 (3%)	38	53
2	L	54/111 (49%)	51 (94%)	3 (6%)	21	29
2	N	94/111 (85%)	91 (97%)	3 (3%)	39	54
2	P	54/111 (49%)	51 (94%)	3 (6%)	21	29
All	All	2084/2392 (87%)	1980 (95%)	104 (5%)	24	34

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	180	LEU
2	L	39	LYS
1	O	220	LEU
1	I	221	LYS
1	K	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	89	HIS
1	I	103	HIS
1	M	103	HIS
2	N	89	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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
3	NO3	F	148	-	1,3,3	3.35	1 (100%)	0,3,3	-	-
8	SAM	K	302	-	24,29,29	1.22	2 (8%)	23,42,42	1.74	2 (8%)
3	NO3	E	255	-	1,3,3	2.90	1 (100%)	0,3,3	-	-
8	SAM	O	302	-	24,29,29	1.29	2 (8%)	23,42,42	1.89	5 (21%)
6	EDO	A	259	-	3,3,3	0.55	0	2,2,2	0.08	0
3	NO3	A	255	-	1,3,3	2.87	1 (100%)	0,3,3	-	-
3	NO3	N	148	-	1,3,3	3.11	1 (100%)	0,3,3	-	-
7	2MM	M	257	-	7,9,10	0.63	0	6,10,12	1.48	1 (16%)
3	NO3	M	255	-	1,3,3	3.28	1 (100%)	0,3,3	-	-
3	NO3	I	256	-	1,3,3	3.15	1 (100%)	0,3,3	-	-
7	2MM	F	149	2	7,9,10	0.73	0	6,10,12	1.41	1 (16%)
5	SAH	M	256	-	24,28,28	1.08	3 (12%)	25,40,40	1.88	4 (16%)
5	SAH	I	259	-	24,28,28	1.10	3 (12%)	25,40,40	1.76	4 (16%)
5	SAH	A	258	-	24,28,28	1.10	3 (12%)	25,40,40	1.86	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	2MM	J	148	2	7,9,10	0.79	0	6,10,12	1.15	1 (16%)
6	EDO	B	150	-	3,3,3	0.49	0	2,2,2	0.32	0
7	2MM	B	149	2	7,9,10	0.74	0	6,10,12	1.16	0
8	SAM	C	302	-	24,29,29	1.44	3 (12%)	23,42,42	2.10	6 (26%)
5	SAH	E	256	-	24,28,28	1.14	2 (8%)	25,40,40	1.88	3 (12%)
3	NO3	I	255	-	1,3,3	3.06	1 (100%)	0,3,3	-	-
3	NO3	B	148	-	1,3,3	3.15	1 (100%)	0,3,3	-	-
8	SAM	G	302	-	24,29,29	1.28	2 (8%)	23,42,42	1.87	4 (17%)

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
5	SAH	I	259	-	-	1/11/31/31	0/3/3/3
7	2MM	B	149	2	-	3/7/10/12	-
7	2MM	M	257	-	-	5/7/10/12	-
8	SAM	K	302	-	-	5/12/33/33	0/3/3/3
5	SAH	A	258	-	-	1/11/31/31	0/3/3/3
8	SAM	C	302	-	-	4/12/33/33	0/3/3/3
8	SAM	O	302	-	-	5/12/33/33	0/3/3/3
5	SAH	E	256	-	-	1/11/31/31	0/3/3/3
7	2MM	F	149	2	-	1/7/10/12	-
7	2MM	J	148	2	-	6/7/10/12	-
6	EDO	B	150	-	-	1/1/1/1	-
5	SAH	M	256	-	-	1/11/31/31	0/3/3/3
6	EDO	A	259	-	-	1/1/1/1	-
8	SAM	G	302	-	-	6/12/33/33	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	O	302	SAM	C2-N3	4.33	1.39	1.32
8	C	302	SAM	C2-N3	4.25	1.38	1.32
8	K	302	SAM	C2-N3	4.03	1.38	1.32
8	G	302	SAM	C2-N3	3.96	1.38	1.32
5	E	256	SAH	C2-N3	3.69	1.38	1.32

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	256	SAH	N3-C2-N1	-7.48	116.98	128.68
5	M	256	SAH	N3-C2-N1	-7.05	117.67	128.68
5	I	259	SAH	N3-C2-N1	-6.35	118.75	128.68
8	K	302	SAM	N3-C2-N1	-6.34	118.78	128.68
8	O	302	SAM	N3-C2-N1	-6.28	118.86	128.68

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	149	2MM	C-CA-CB-CG
7	J	148	2MM	C-CA-CB-CG
7	J	148	2MM	N-CA-CB-CG
7	J	148	2MM	CB-CA-N-CN2
7	M	257	2MM	C-CA-CB-CG

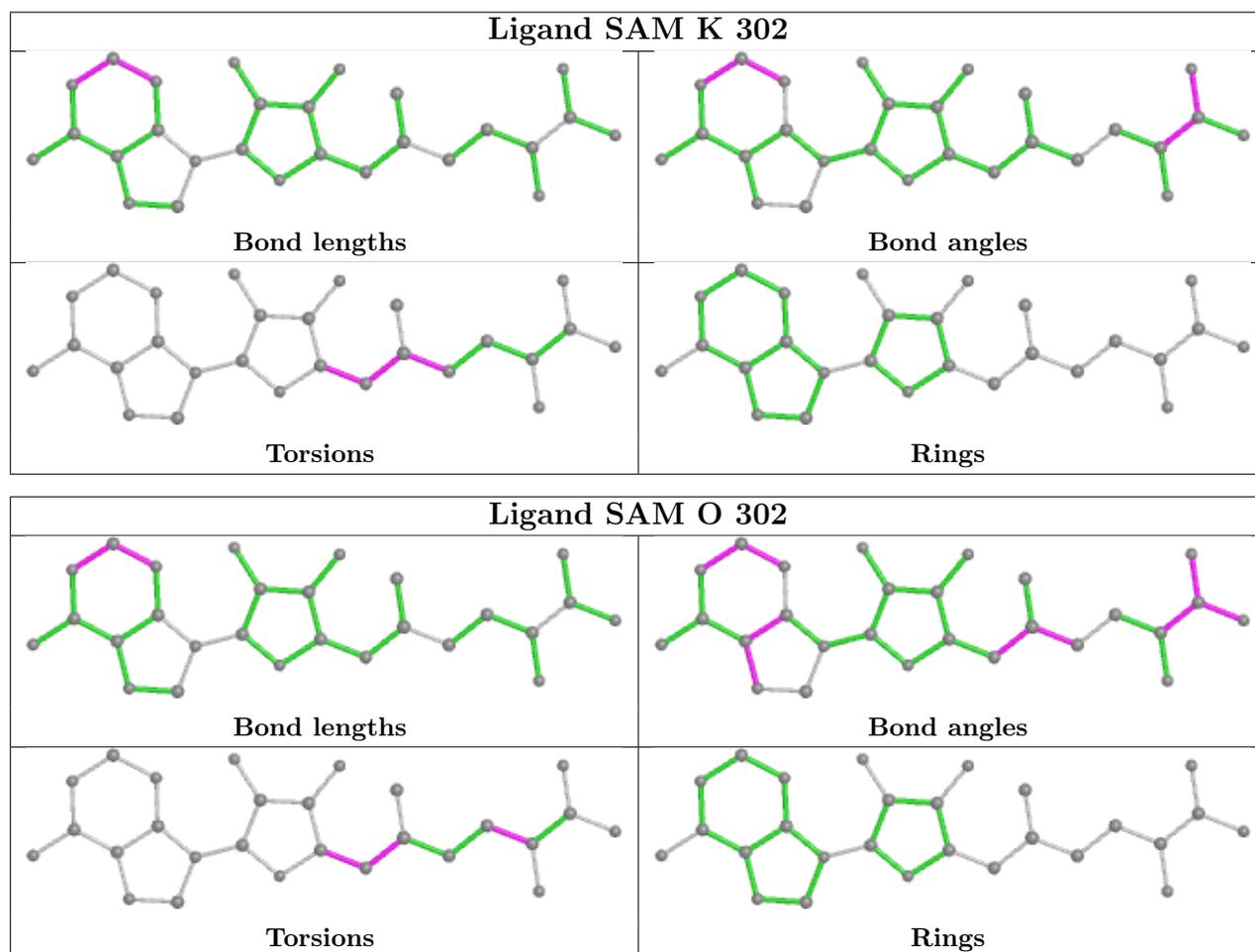
There are no ring outliers.

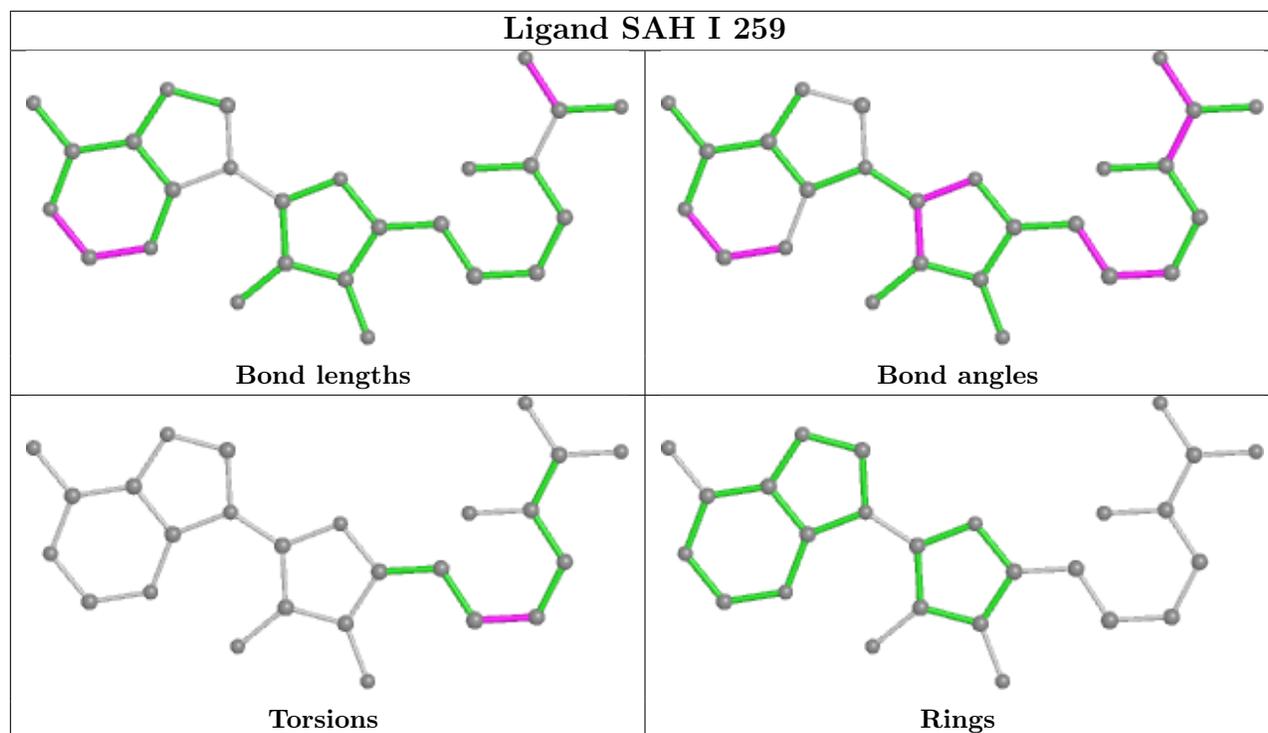
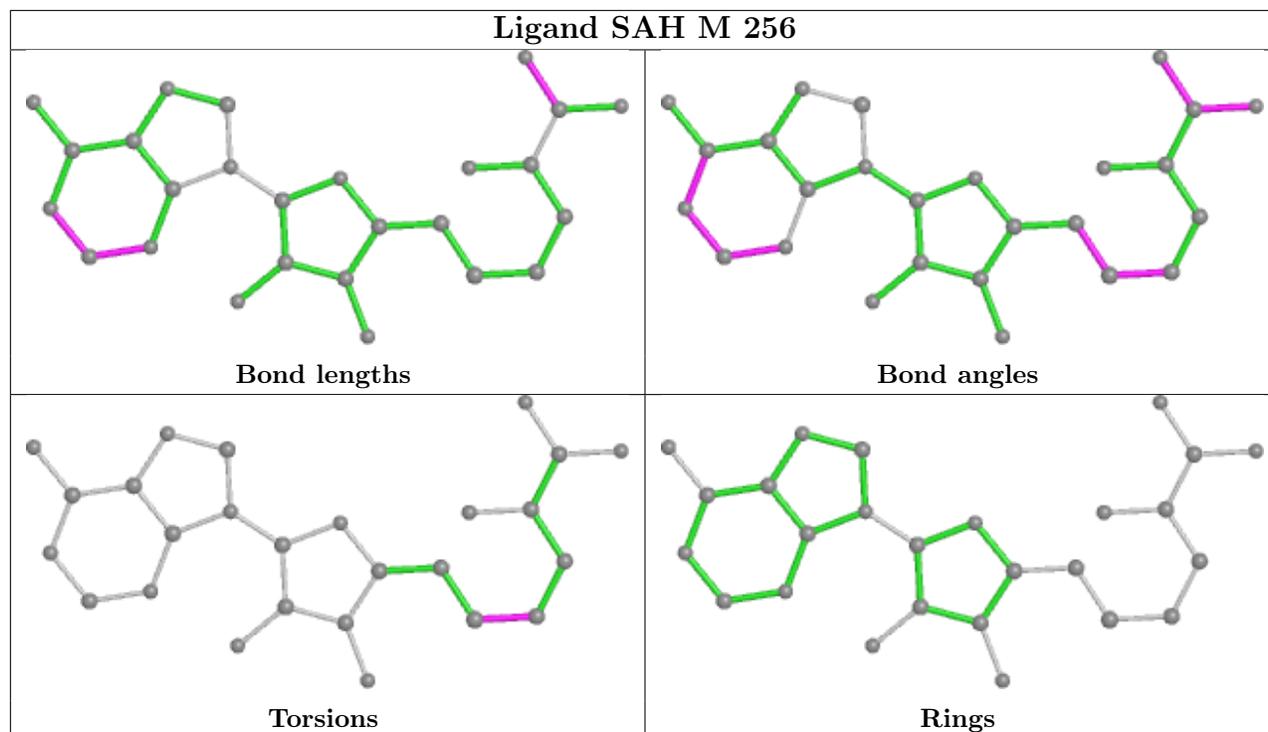
10 monomers are involved in 32 short contacts:

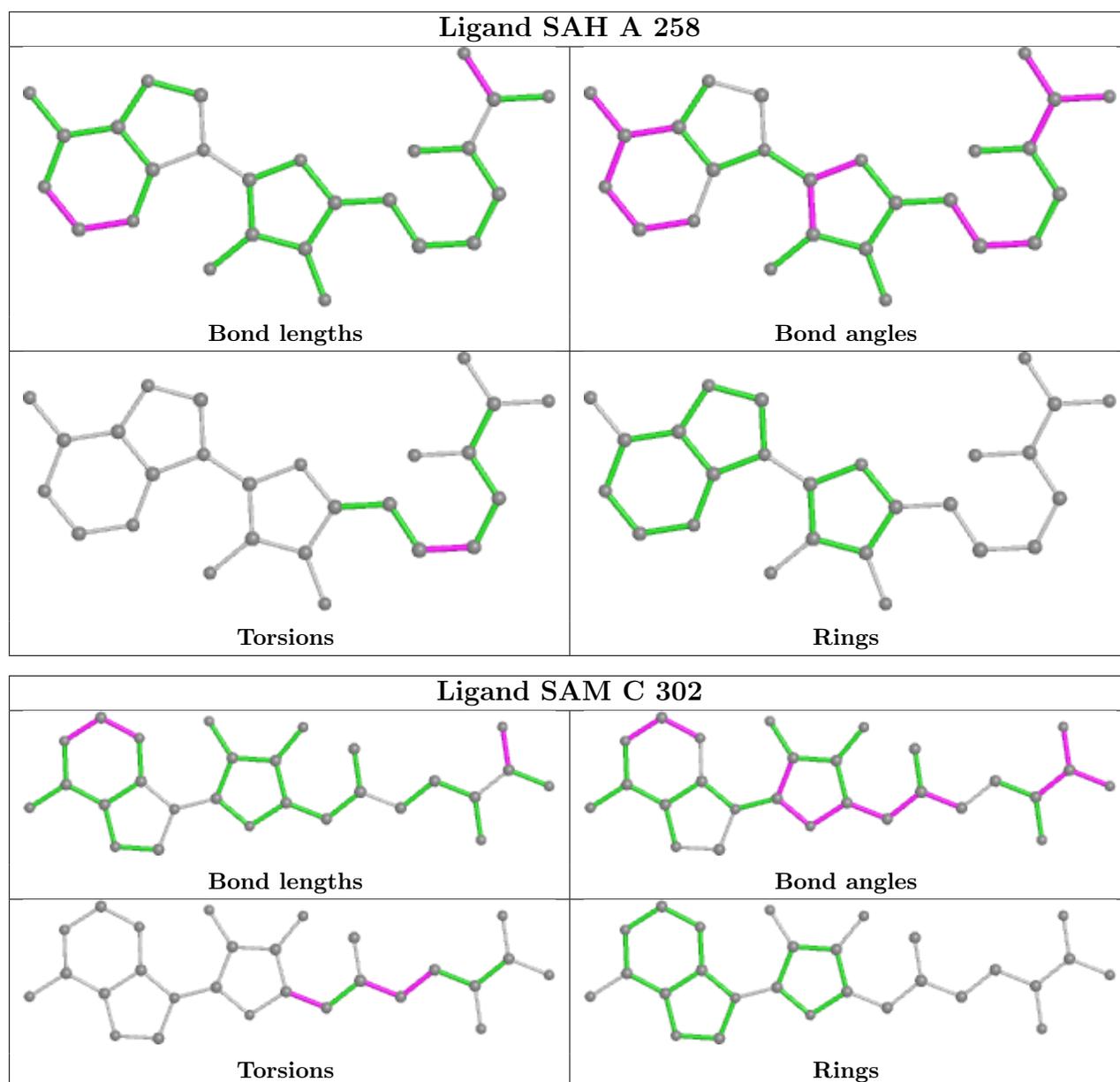
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	148	NO3	1	0
8	K	302	SAM	4	0
8	O	302	SAM	5	0
6	A	259	EDO	1	0
7	M	257	2MM	9	0
7	F	149	2MM	4	0
7	J	148	2MM	1	0
7	B	149	2MM	2	0
8	C	302	SAM	3	0
8	G	302	SAM	2	0

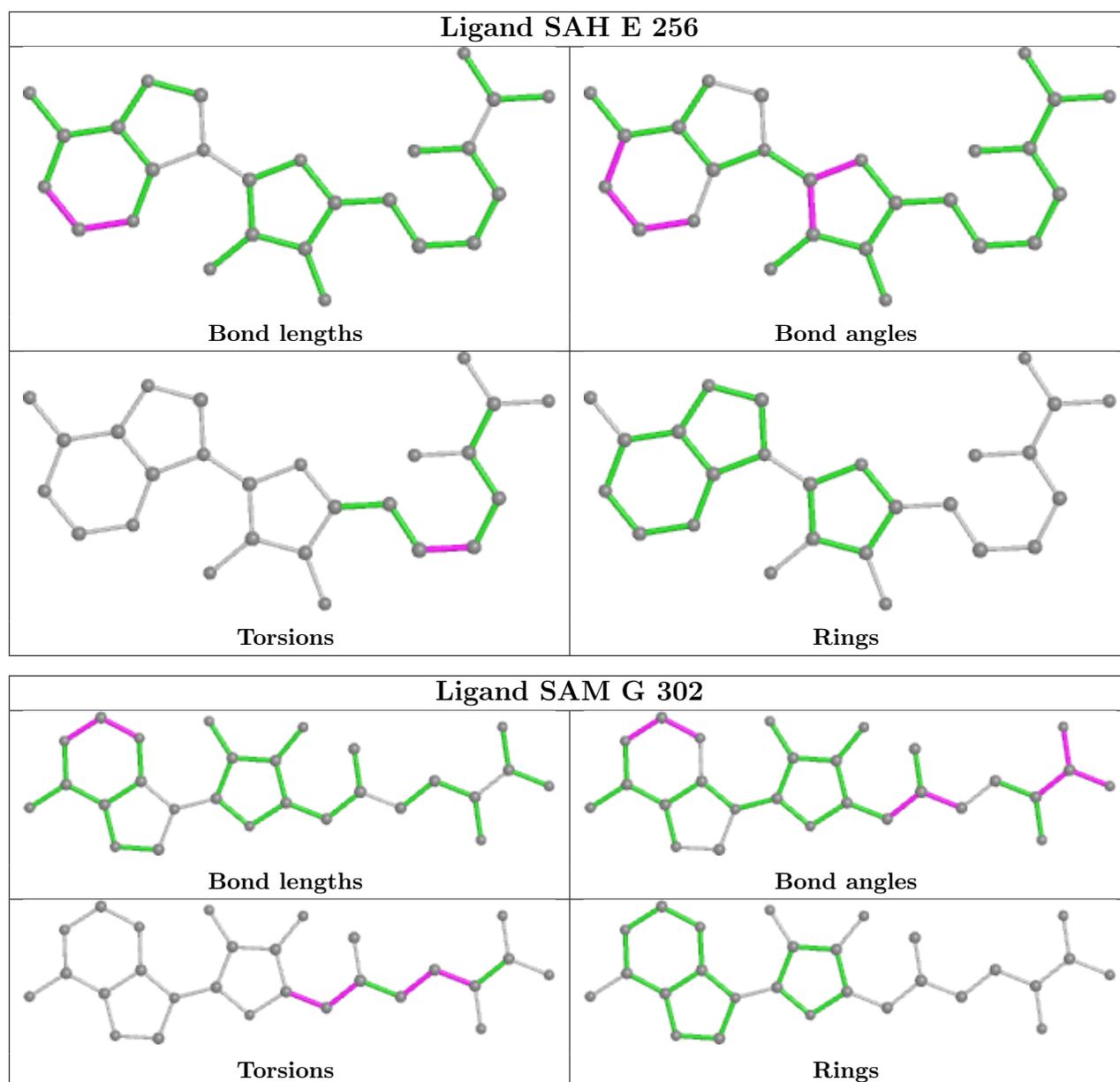
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

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	254/254 (100%)	0.36	1 (0%) 92 95	19, 28, 43, 56	1 (0%)
1	C	250/254 (98%)	0.82	14 (5%) 24 30	23, 32, 67, 70	2 (0%)
1	E	254/254 (100%)	0.47	3 (1%) 79 83	20, 29, 45, 59	0
1	G	251/254 (98%)	0.64	10 (3%) 38 45	22, 32, 66, 70	2 (0%)
1	I	254/254 (100%)	0.24	0 100 100	25, 32, 45, 57	0
1	K	250/254 (98%)	0.80	34 (13%) 3 4	28, 38, 81, 83	2 (0%)
1	M	254/254 (100%)	0.21	1 (0%) 92 95	25, 33, 48, 62	0
1	O	250/254 (98%)	0.78	35 (14%) 2 4	28, 37, 78, 81	2 (0%)
2	B	126/147 (85%)	0.77	15 (11%) 4 6	22, 39, 80, 92	0
2	D	72/147 (48%)	1.71	26 (36%) 0 0	62, 70, 86, 90	2 (2%)
2	F	130/147 (88%)	0.94	18 (13%) 2 4	23, 48, 92, 98	0
2	H	71/147 (48%)	1.09	7 (9%) 7 10	62, 68, 85, 90	2 (2%)
2	J	127/147 (86%)	0.73	11 (8%) 10 14	25, 42, 83, 92	0
2	L	72/147 (48%)	2.46	40 (55%) 0 0	76, 84, 100, 100	2 (2%)
2	N	130/147 (88%)	0.73	18 (13%) 2 4	27, 50, 91, 100	0
2	P	72/147 (48%)	2.54	35 (48%) 0 0	78, 82, 98, 100	2 (2%)
All	All	2817/3208 (87%)	0.73	268 (9%) 8 11	19, 35, 83, 100	17 (0%)

The worst 5 of 268 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	10	LEU	9.6
2	P	4	VAL	9.4
2	P	71	THR	8.7
2	B	125	ARG	8.7
2	B	126	MET	7.8

## 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](#)

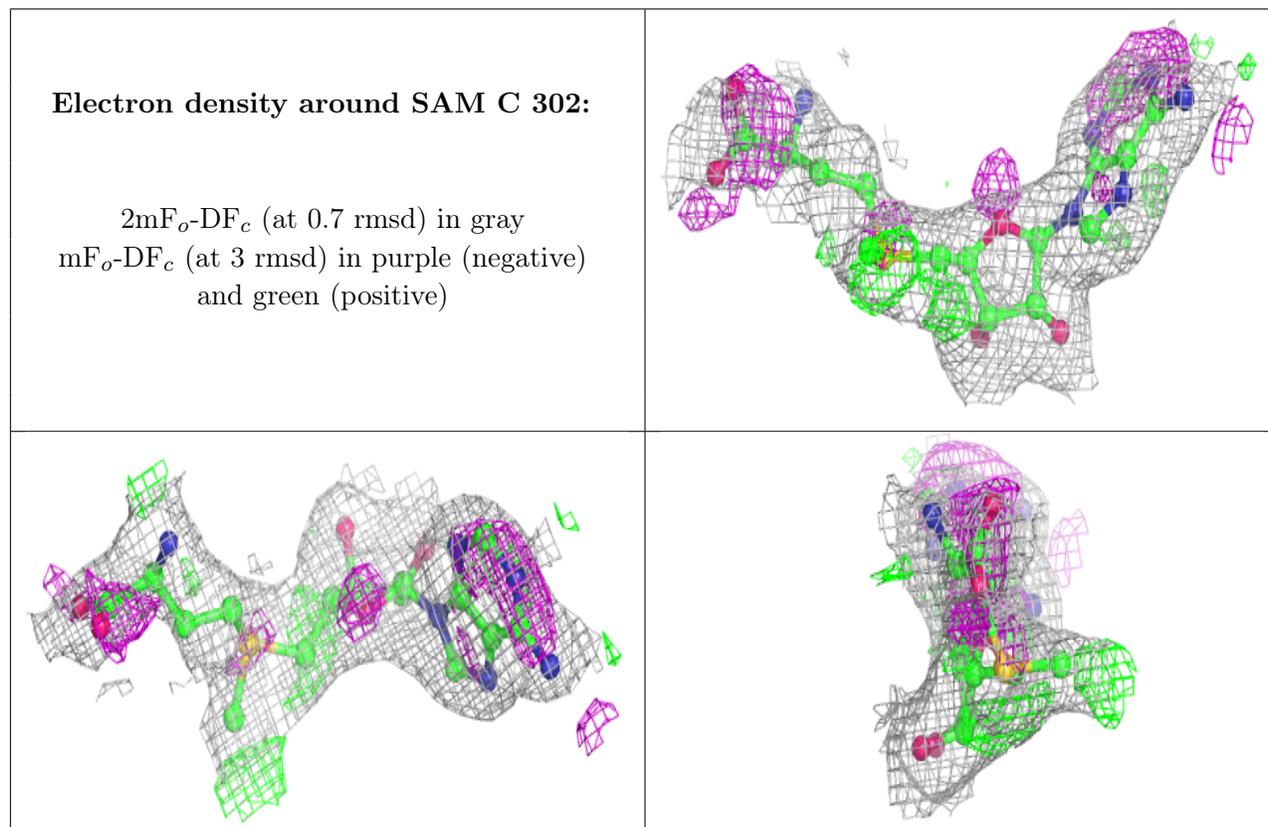
There are no monosaccharides in this entry.

## 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.

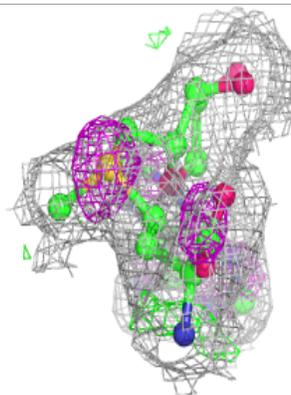
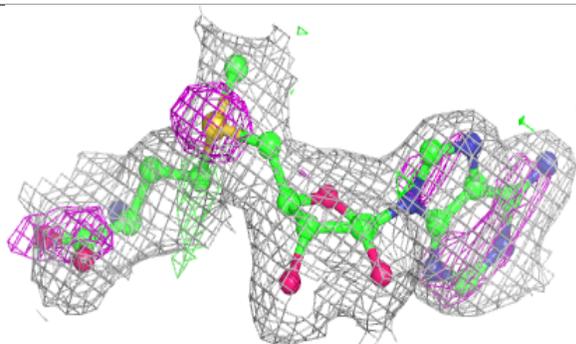
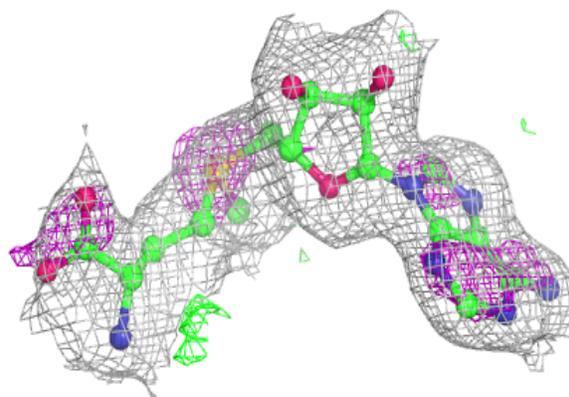
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	B	150	4/4	0.39	0.24	81,81,82,82	0
6	EDO	A	259	4/4	0.83	0.29	74,74,74,74	0
4	CL	I	257	1/1	0.84	0.10	53,53,53,53	0
8	SAM	C	302	27/27	0.85	0.19	31,35,56,57	0
8	SAM	O	302	27/27	0.85	0.18	36,39,56,58	0
4	CL	I	258	1/1	0.87	0.12	48,48,48,48	0
8	SAM	G	302	27/27	0.88	0.16	30,33,54,55	0
7	2MM	F	149	10/11	0.88	0.14	26,28,38,38	0
5	SAH	I	259	26/26	0.91	0.13	22,25,28,29	0
3	NO3	F	148	4/4	0.91	0.15	37,38,38,38	0
7	2MM	J	148	10/11	0.91	0.15	27,30,38,39	0
7	2MM	M	257	10/11	0.92	0.21	37,39,40,43	0
7	2MM	B	149	10/11	0.92	0.14	23,25,37,37	0
3	NO3	N	148	4/4	0.92	0.30	38,39,39,39	0
8	SAM	K	302	27/27	0.92	0.18	34,41,54,57	0
3	NO3	I	256	4/4	0.92	0.17	25,26,26,27	0
4	CL	A	257	1/1	0.93	0.06	47,47,47,47	0
3	NO3	M	255	4/4	0.94	0.20	30,30,31,33	0
5	SAH	M	256	26/26	0.94	0.14	21,27,28,29	0
5	SAH	E	256	26/26	0.94	0.11	18,22,24,24	0
3	NO3	I	255	4/4	0.95	0.14	32,32,32,32	0
3	NO3	E	255	4/4	0.95	0.23	23,24,25,27	0
3	NO3	A	255	4/4	0.96	0.15	27,27,28,29	0
5	SAH	A	258	26/26	0.96	0.08	17,21,23,25	0
4	CL	A	256	1/1	0.96	0.09	47,47,47,47	0
3	NO3	B	148	4/4	0.97	0.15	30,30,31,31	0

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

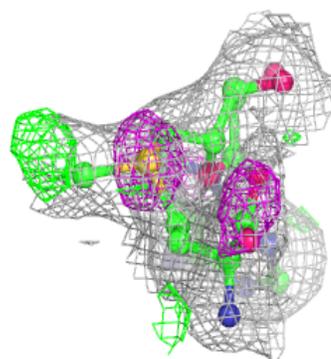
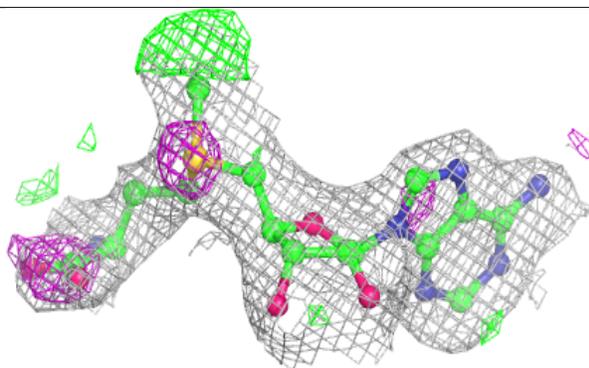
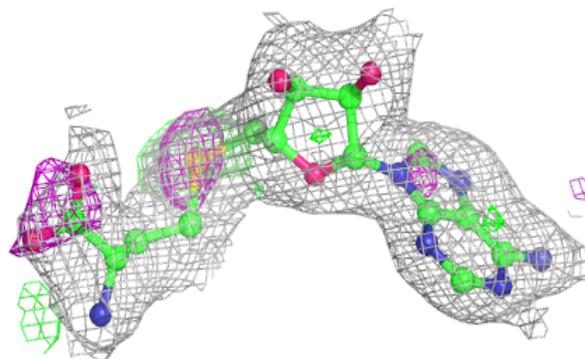


**Electron density around SAM O 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

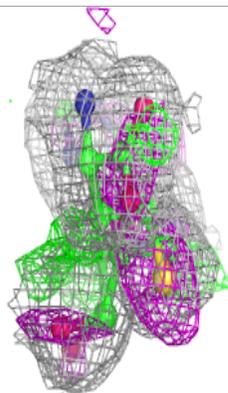
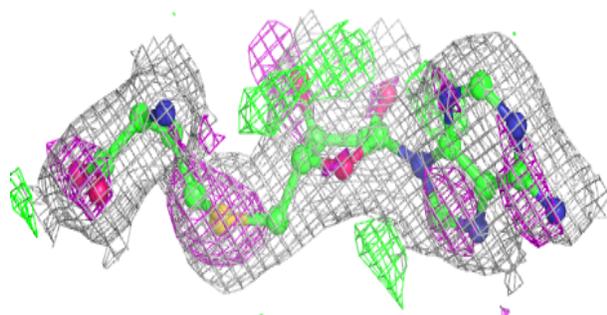
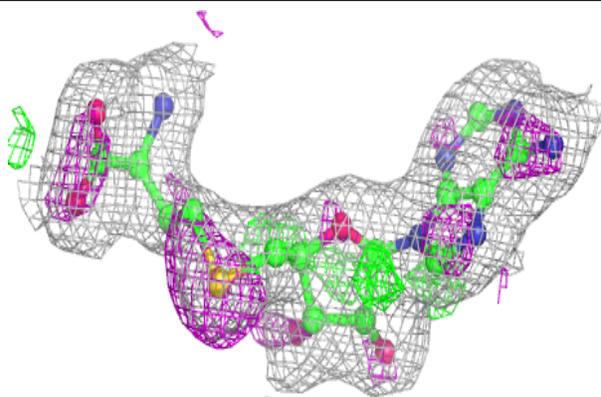
**Electron density around SAM G 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

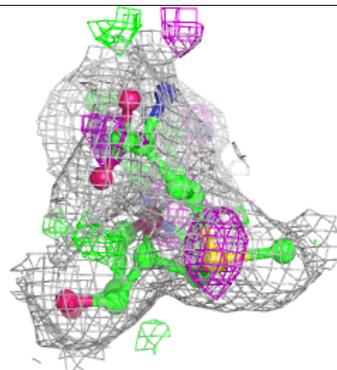
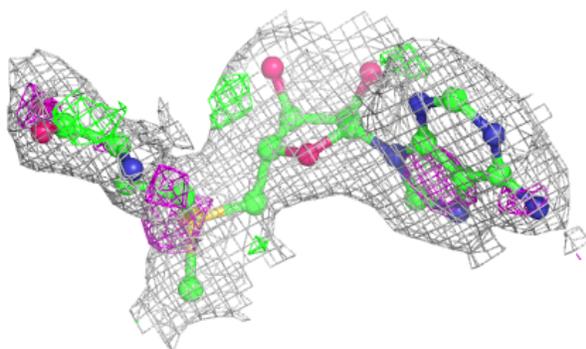
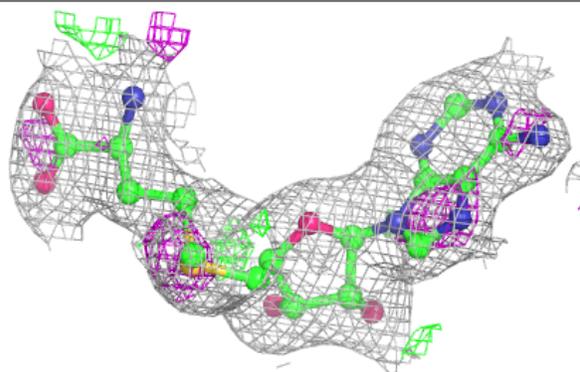


**Electron density around SAH I 259:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

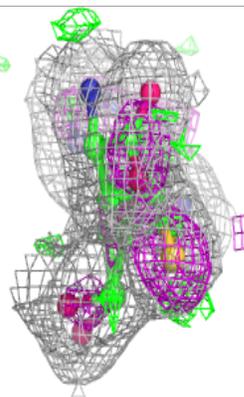
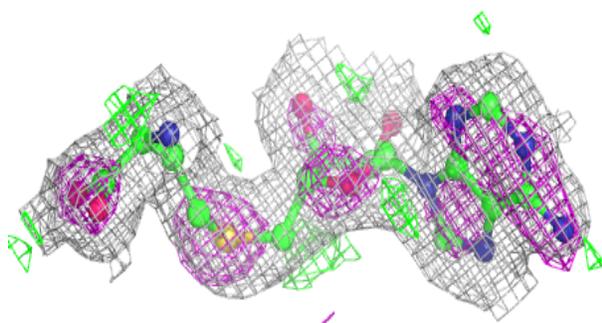
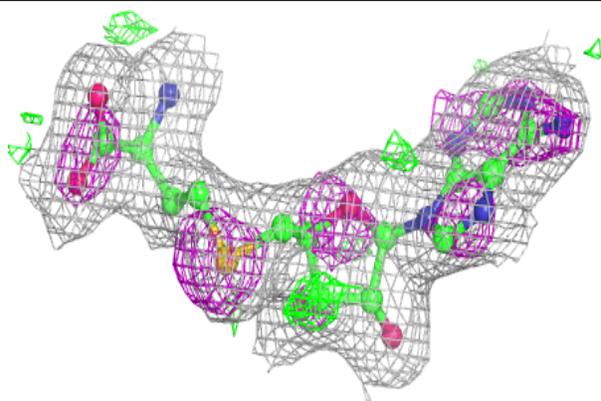
**Electron density around SAM K 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

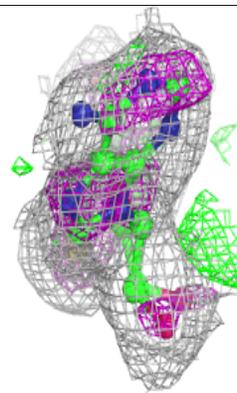
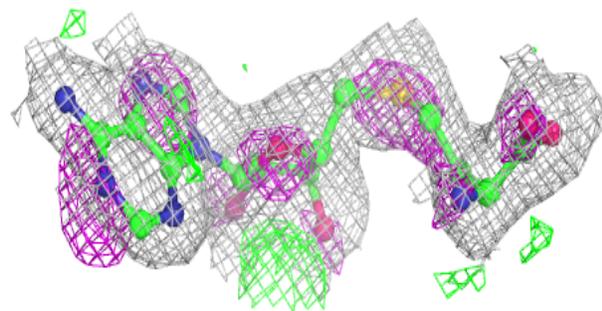
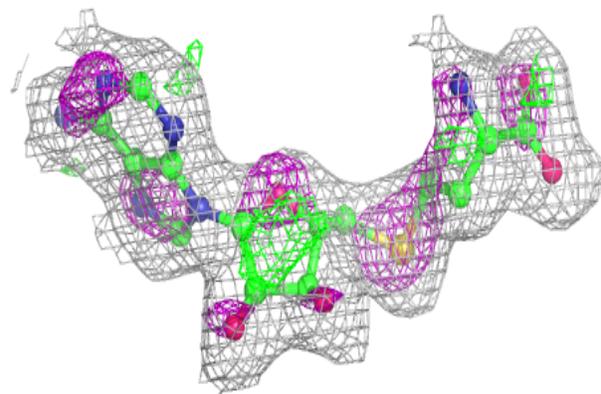


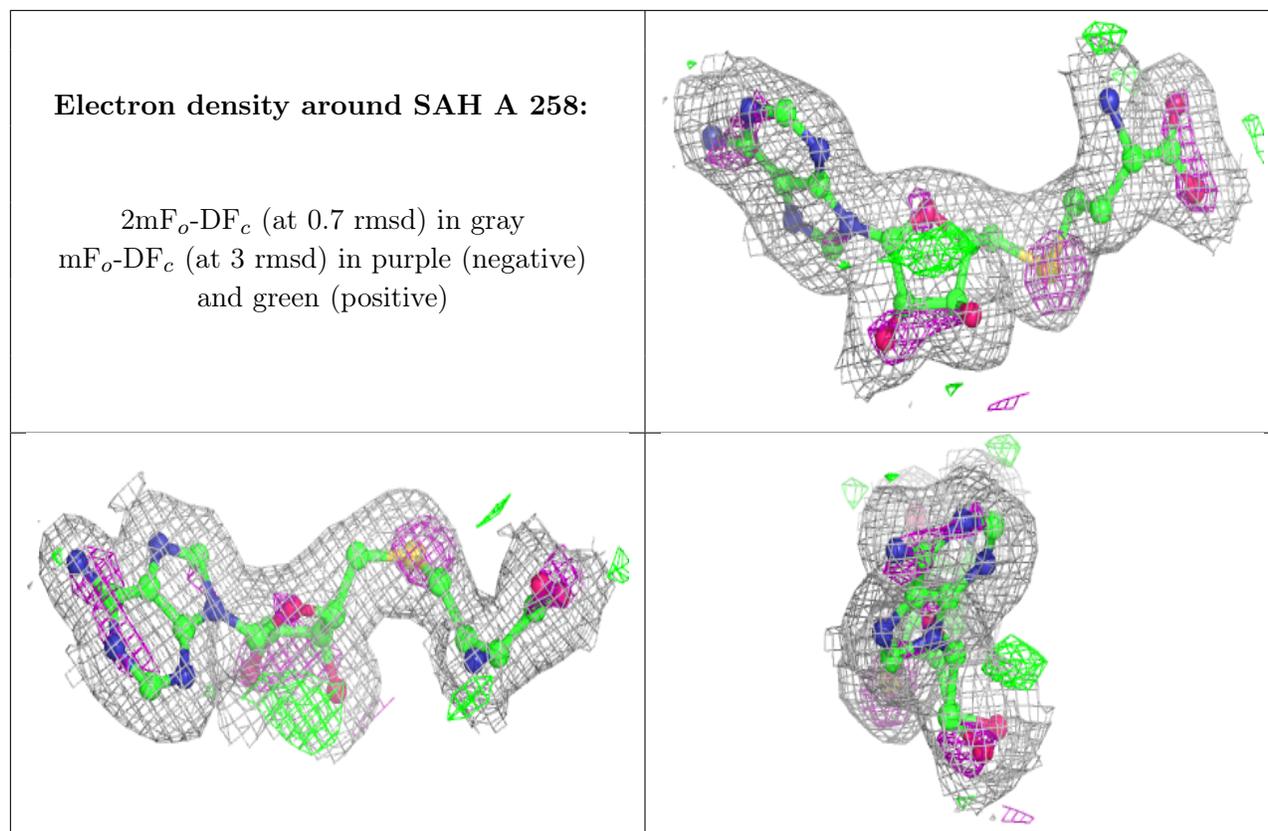
**Electron density around SAH M 256:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around SAH E 256:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.