



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2022 – 06:04 PM JST

PDB ID : 7VRS  
Title : The complex of Acyltransferase and Acyl Carrier Protein Domains from module 9 of Salinomycin Polyketide Synthase  
Authors : Feng, Y.; Zheng, J.  
Deposited on : 2021-10-24  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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 : 2.28.1  
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) : 2.28.1

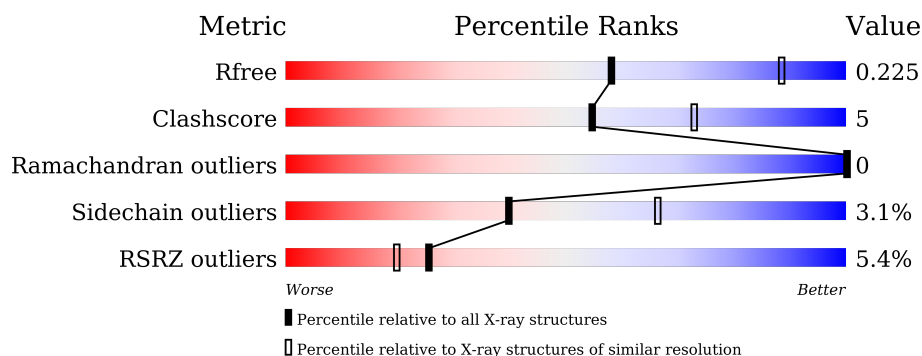
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	466	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>82%</span> <span>13%</span> <span>• 5%</span> </div> </div>
1	B	466	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>84%</span> <span>10%</span> <span>• 5%</span> </div> </div>
2	C	107	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>36%</span> <span>68%</span> <span>11%</span> <span>• 20%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7319 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 Type I modular polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3255	2054	569	628	4			
1	B	444	Total	C	N	O	S	0	0	0
			3255	2054	569	628	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP H1ZZT7
A	-20	GLY	-	expression tag	UNP H1ZZT7
A	-19	SER	-	expression tag	UNP H1ZZT7
A	-18	SER	-	expression tag	UNP H1ZZT7
A	-17	HIS	-	expression tag	UNP H1ZZT7
A	-16	HIS	-	expression tag	UNP H1ZZT7
A	-15	HIS	-	expression tag	UNP H1ZZT7
A	-14	HIS	-	expression tag	UNP H1ZZT7
A	-13	HIS	-	expression tag	UNP H1ZZT7
A	-12	HIS	-	expression tag	UNP H1ZZT7
A	-11	SER	-	expression tag	UNP H1ZZT7
A	-10	SER	-	expression tag	UNP H1ZZT7
A	-9	GLY	-	expression tag	UNP H1ZZT7
A	-8	LEU	-	expression tag	UNP H1ZZT7
A	-7	VAL	-	expression tag	UNP H1ZZT7
A	-6	PRO	-	expression tag	UNP H1ZZT7
A	-5	ARG	-	expression tag	UNP H1ZZT7
A	-4	GLY	-	expression tag	UNP H1ZZT7
A	-3	SER	-	expression tag	UNP H1ZZT7
A	-2	HIS	-	expression tag	UNP H1ZZT7
A	-1	MET	-	expression tag	UNP H1ZZT7
A	190	CYS	SER	engineered mutation	UNP H1ZZT7
A	298	SER	CYS	engineered mutation	UNP H1ZZT7
A	347	SER	CYS	engineered mutation	UNP H1ZZT7
B	-21	MET	-	initiating methionine	UNP H1ZZT7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	GLY	-	expression tag	UNP H1ZZT7
B	-19	SER	-	expression tag	UNP H1ZZT7
B	-18	SER	-	expression tag	UNP H1ZZT7
B	-17	HIS	-	expression tag	UNP H1ZZT7
B	-16	HIS	-	expression tag	UNP H1ZZT7
B	-15	HIS	-	expression tag	UNP H1ZZT7
B	-14	HIS	-	expression tag	UNP H1ZZT7
B	-13	HIS	-	expression tag	UNP H1ZZT7
B	-12	HIS	-	expression tag	UNP H1ZZT7
B	-11	SER	-	expression tag	UNP H1ZZT7
B	-10	SER	-	expression tag	UNP H1ZZT7
B	-9	GLY	-	expression tag	UNP H1ZZT7
B	-8	LEU	-	expression tag	UNP H1ZZT7
B	-7	VAL	-	expression tag	UNP H1ZZT7
B	-6	PRO	-	expression tag	UNP H1ZZT7
B	-5	ARG	-	expression tag	UNP H1ZZT7
B	-4	GLY	-	expression tag	UNP H1ZZT7
B	-3	SER	-	expression tag	UNP H1ZZT7
B	-2	HIS	-	expression tag	UNP H1ZZT7
B	-1	MET	-	expression tag	UNP H1ZZT7
B	190	CYS	SER	engineered mutation	UNP H1ZZT7
B	298	SER	CYS	engineered mutation	UNP H1ZZT7
B	347	SER	CYS	engineered mutation	UNP H1ZZT7

- Molecule 2 is a protein called Type I modular polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	86	Total	C	N	O	S	0	0	0
			633	398	116	118	1			

There are 21 discrepancies between the modelled and reference sequences:

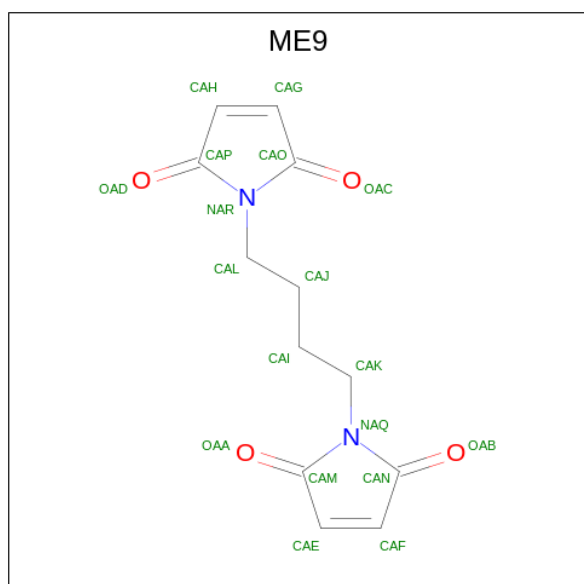
Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	initiating methionine	UNP H1ZZT7
C	-17	GLY	-	expression tag	UNP H1ZZT7
C	-16	SER	-	expression tag	UNP H1ZZT7
C	-15	SER	-	expression tag	UNP H1ZZT7
C	-14	HIS	-	expression tag	UNP H1ZZT7
C	-13	HIS	-	expression tag	UNP H1ZZT7
C	-12	HIS	-	expression tag	UNP H1ZZT7
C	-11	HIS	-	expression tag	UNP H1ZZT7
C	-10	HIS	-	expression tag	UNP H1ZZT7

*Continued on next page...*

Continued from previous page...

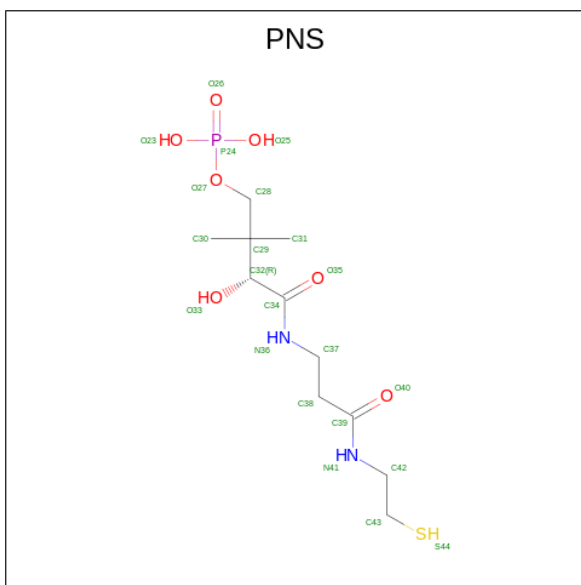
Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	HIS	-	expression tag	UNP H1ZZT7
C	-8	SER	-	expression tag	UNP H1ZZT7
C	-7	SER	-	expression tag	UNP H1ZZT7
C	-6	GLY	-	expression tag	UNP H1ZZT7
C	-5	LEU	-	expression tag	UNP H1ZZT7
C	-4	VAL	-	expression tag	UNP H1ZZT7
C	-3	PRO	-	expression tag	UNP H1ZZT7
C	-2	ARG	-	expression tag	UNP H1ZZT7
C	-1	GLY	-	expression tag	UNP H1ZZT7
C	0	SER	-	expression tag	UNP H1ZZT7
C	1	HIS	-	expression tag	UNP H1ZZT7
C	2	MET	-	expression tag	UNP H1ZZT7

- Molecule 3 is 1,1'-butane-1,4-diylbis(1H-pyrrole-2,5-dione) (three-letter code: ME9) (formula: C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	12	2	4		
3	B	1	Total	C	N	O	0	0
			18	12	2	4		

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

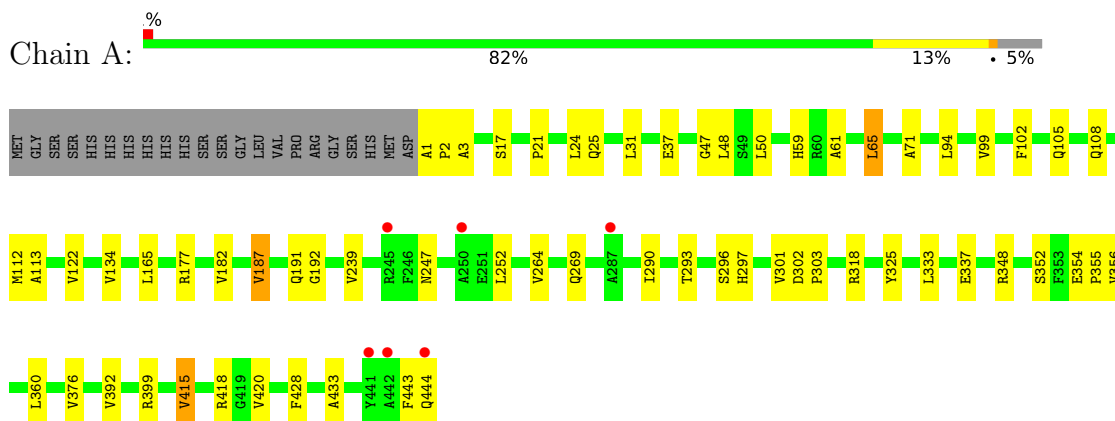
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	68	Total O 68 68	0	0
5	B	51	Total O 51 51	0	0

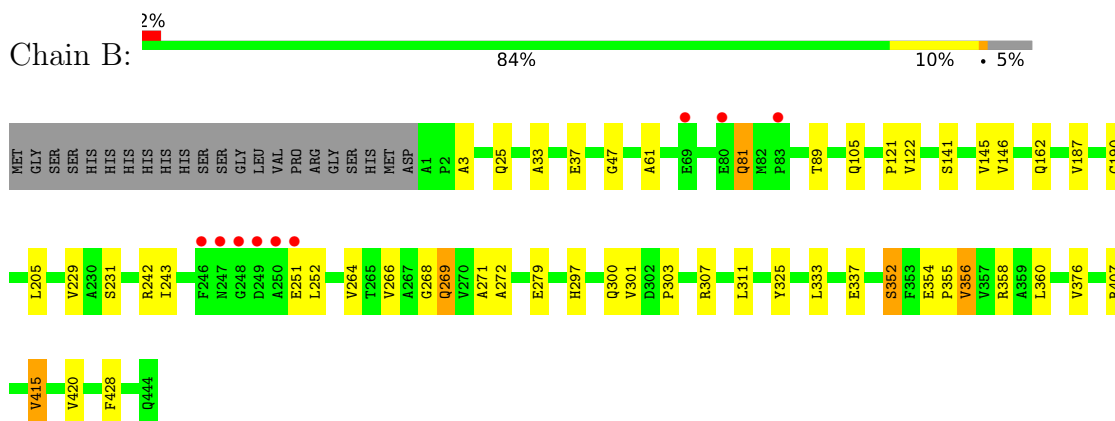
### 3 Residue-property plots

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.

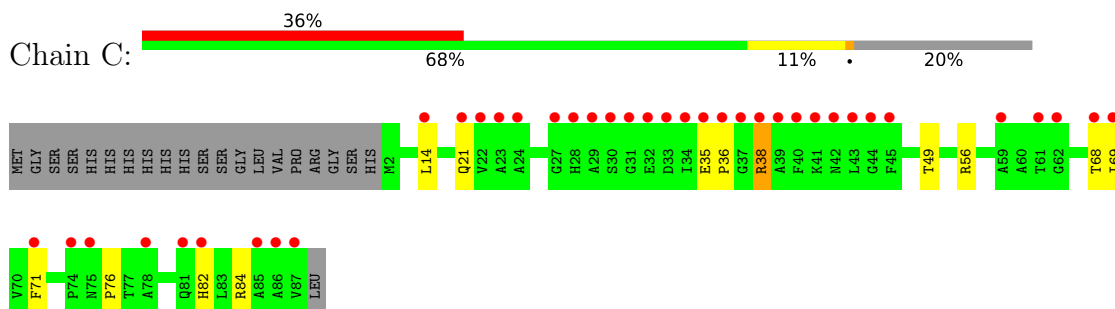
#### • Molecule 1: Type I modular polyketide synthase



#### • Molecule 1: Type I modular polyketide synthase



#### • Molecule 2: Type I modular polyketide synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.61Å 102.06Å 150.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.60 47.33 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.38-2.60) 99.0 (47.33-2.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.186 , 0.225 0.194 , 0.225	Depositor DCC
$R_{free}$ test set	1816 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ME9, PNS

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	0.72	0/3317	0.81	0/4527
1	B	0.74	0/3317	0.79	0/4527
2	C	0.67	0/644	0.75	0/876
All	All	0.72	0/7278	0.79	0/9930

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3255	0	3220	40	0
1	B	3255	0	3220	27	0
2	C	633	0	636	9	0
3	A	18	0	10	1	0
3	B	18	0	11	0	0
4	C	21	0	20	0	0
5	A	68	0	0	0	0
5	B	51	0	0	0	0
All	All	7319	0	7117	75	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 5.

All (75) 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:A:239:VAL:HG21	1:A:264:VAL:HG11	1.57	0.86
1:A:239:VAL:HG21	1:A:264:VAL:CG1	2.19	0.73
1:A:247:ASN:HB2	1:A:252:LEU:H	1.55	0.71
1:A:296:SER:OG	1:A:297:HIS:CD2	2.45	0.70
1:A:301:VAL:HG22	1:A:348:ARG:HD3	1.74	0.70
1:B:269:GLN:HE21	1:B:272:ALA:H	1.40	0.70
1:A:415:VAL:HG13	1:A:420:VAL:HB	1.73	0.68
1:A:354:GLU:HB3	1:A:355:PRO:HD3	1.75	0.67
1:B:352:SER:O	1:B:356:VAL:HG13	1.94	0.67
1:B:415:VAL:HG13	1:B:420:VAL:HB	1.78	0.66
1:B:105:GLN:NE2	1:B:162:GLN:HE21	1.95	0.65
1:A:415:VAL:HG13	1:A:420:VAL:CB	2.29	0.63
1:A:3:ALA:O	1:A:122:VAL:HG23	1.99	0.62
1:A:247:ASN:CB	1:A:252:LEU:H	2.13	0.62
1:B:187:VAL:HG11	1:B:360:LEU:HD11	1.85	0.58
1:B:251:GLU:O	1:B:251:GLU:HG3	2.04	0.57
1:A:65:LEU:HD13	1:A:71:ALA:HB2	1.87	0.56
1:A:187:VAL:HG11	1:A:360:LEU:HD11	1.90	0.53
1:A:301:VAL:CG2	1:A:348:ARG:HD3	2.39	0.52
1:A:296:SER:OG	1:A:297:HIS:HD2	1.90	0.52
1:A:112:MET:O	1:A:113:ALA:HB3	2.08	0.52
1:B:105:GLN:HE21	1:B:162:GLN:HE21	1.56	0.52
1:B:407:ARG:O	1:B:407:ARG:HD3	2.11	0.51
2:C:21:GLN:HE21	2:C:56:ARG:HD3	1.77	0.50
1:A:3:ALA:C	1:A:122:VAL:HG23	2.32	0.50
1:B:354:GLU:HB3	1:B:355:PRO:HD3	1.94	0.48
1:A:31:LEU:HD21	1:A:50:LEU:HD11	1.94	0.48
1:B:3:ALA:C	1:B:122:VAL:HG23	2.34	0.48
2:C:14:LEU:CD1	2:C:84:ARG:HG2	2.43	0.48
1:A:239:VAL:CG2	1:A:264:VAL:HG11	2.34	0.48
2:C:68:THR:HA	2:C:71:PHE:HD2	1.79	0.47
1:B:187:VAL:HG12	1:B:325:TYR:HB2	1.97	0.47
1:B:190:CYS:HB3	1:B:297:HIS:CE1	2.50	0.47
1:B:333:LEU:HD22	1:B:337:GLU:HG3	1.98	0.46
1:A:302:ASP:N	1:A:303:PRO:CD	2.79	0.46
1:A:24:LEU:HD21	1:A:61:ALA:HB2	1.98	0.46
1:B:354:GLU:OE1	1:B:358:ARG:NH1	2.45	0.46
1:B:25:GLN:NE2	1:B:81:GLN:HG2	2.30	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HD22	1:A:433:ALA:HB3	1.98	0.45
1:A:301:VAL:HG22	1:A:348:ARG:CD	2.45	0.45
1:A:105:GLN:HB2	3:A:501:ME9:HAJ	1.99	0.45
1:A:102:PHE:O	1:A:192:GLY:HA3	2.17	0.45
1:B:205:LEU:HD12	1:B:205:LEU:HA	1.79	0.45
1:B:229:VAL:HA	1:B:266:VAL:O	2.16	0.45
1:A:333:LEU:HD22	1:A:337:GLU:HG3	1.99	0.44
1:A:290:ILE:HB	1:A:293:THR:HG21	1.99	0.43
1:A:1:ALA:N	1:A:2:PRO:HD2	2.33	0.43
1:B:141:SER:O	1:B:145:VAL:HG23	2.18	0.43
1:B:300:GLN:O	1:B:303:PRO:HD2	2.19	0.43
1:A:352:SER:O	1:A:356:VAL:HG13	2.19	0.43
1:B:269:GLN:NE2	1:B:271:ALA:HB3	2.33	0.43
2:C:35:GLU:HB2	2:C:38:ARG:HB2	2.00	0.43
1:A:177:ARG:HG3	1:A:182:VAL:HG12	2.00	0.43
1:A:17:SER:HA	1:A:59:HIS:O	2.19	0.43
1:B:3:ALA:O	1:B:121:PRO:HD2	2.19	0.42
1:B:33:ALA:O	1:B:37:GLU:HG2	2.19	0.42
1:A:108:GLN:HB3	1:A:165:LEU:HD21	2.00	0.42
1:B:47:GLY:HA3	1:B:428:PHE:CZ	2.54	0.42
1:A:399:ARG:NH2	2:C:49:THR:HG23	2.34	0.42
2:C:21:GLN:NE2	2:C:56:ARG:HD3	2.35	0.42
1:A:187:VAL:CG1	1:A:325:TYR:HB2	2.49	0.42
1:A:21:PRO:O	1:A:25:GLN:HG3	2.19	0.42
1:B:307:ARG:O	1:B:311:LEU:HB2	2.20	0.42
2:C:69:ILE:HD11	2:C:82:HIS:HD2	1.84	0.41
1:A:47:GLY:HA3	1:A:428:PHE:CZ	2.55	0.41
1:B:252:LEU:O	1:B:268:GLY:HA3	2.20	0.41
1:A:94:LEU:HD12	1:A:418:ARG:HB3	2.02	0.41
1:A:415:VAL:CG1	1:A:420:VAL:HB	2.46	0.41
1:A:443:PHE:O	1:A:444:GLN:HB2	2.21	0.41
1:B:61:ALA:HB2	1:B:89:THR:HG22	2.03	0.41
2:C:21:GLN:NE2	2:C:21:GLN:HA	2.35	0.41
1:A:99:VAL:HG22	1:A:187:VAL:HG22	2.03	0.40
1:A:182:VAL:O	1:A:182:VAL:HG23	2.22	0.40
1:B:242:ARG:HD2	1:B:279:GLU:OE2	2.21	0.40
2:C:36:PRO:O	2:C:76:PRO:HD2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	442/466 (95%)	425 (96%)	17 (4%)	0	100	100
1	B	442/466 (95%)	431 (98%)	11 (2%)	0	100	100
2	C	84/107 (78%)	83 (99%)	1 (1%)	0	100	100
All	All	968/1039 (93%)	939 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/346 (94%)	317 (97%)	10 (3%)	40	66
1	B	327/346 (94%)	316 (97%)	11 (3%)	37	63
2	C	62/80 (78%)	61 (98%)	1 (2%)	62	82
All	All	716/772 (93%)	694 (97%)	22 (3%)	40	66

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	65	LEU
1	A	134	VAL
1	A	187	VAL
1	A	191	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	269	GLN
1	A	318	ARG
1	A	376	VAL
1	A	392	VAL
1	A	415	VAL
1	B	81	GLN
1	B	146	VAL
1	B	231	SER
1	B	243	ILE
1	B	264	VAL
1	B	269	GLN
1	B	301	VAL
1	B	352	SER
1	B	356	VAL
1	B	376	VAL
1	B	415	VAL
2	C	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	210	GLN
1	A	297	HIS
1	B	25	GLN
1	B	81	GLN
1	B	105	GLN
1	B	189	HIS
1	B	269	GLN
1	B	297	HIS
1	B	395	GLN
1	B	444	GLN
2	C	21	GLN
2	C	82	HIS

### 5.3.3 RNA ⓘ

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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ME9	A	501	4,1	19,19,19	0.77	0	26,26,26	1.15	4 (15%)
3	ME9	B	501	1	19,19,19	0.70	0	26,26,26	1.18	2 (7%)
4	PNS	C	101	2,3	13,20,21	0.55	0	18,26,29	1.04	1 (5%)

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
3	ME9	A	501	4,1	-	3/7/33/33	0/2/2/2
3	ME9	B	501	1	-	4/7/33/33	0/2/2/2
4	PNS	C	101	2,3	-	8/24/26/27	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	ME9	CAL-NAR-CAP	-3.67	119.84	124.88
3	A	501	ME9	CAF-CAE-CAM	-3.30	102.86	108.67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	ME9	CAF-CAN-NAQ	-2.92	103.32	106.07
3	B	501	ME9	CAP-NAR-CAO	-2.68	107.78	109.95
4	C	101	PNS	C37-C38-C39	2.49	116.50	112.36
3	A	501	ME9	CAE-CAF-CAN	-2.31	104.60	108.67
3	A	501	ME9	CAN-NAQ-CAM	-2.00	108.33	109.95

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	ME9	CAJ-CAL-NAR-CAP
4	C	101	PNS	O27-C28-C29-C30
4	C	101	PNS	O27-C28-C29-C31
4	C	101	PNS	O27-C28-C29-C32
4	C	101	PNS	N36-C37-C38-C39
4	C	101	PNS	N41-C42-C43-S44
4	C	101	PNS	C38-C39-N41-C42
3	A	501	ME9	CAI-CAK-NAQ-CAM
4	C	101	PNS	O40-C39-N41-C42
3	B	501	ME9	CAI-CAJ-CAL-NAR
3	A	501	ME9	CAI-CAK-NAQ-CAN
3	B	501	ME9	CAJ-CAL-NAR-CAO
3	A	501	ME9	CAK-CAI-CAJ-CAL
3	B	501	ME9	CAK-CAI-CAJ-CAL
4	C	101	PNS	C37-C38-C39-O40

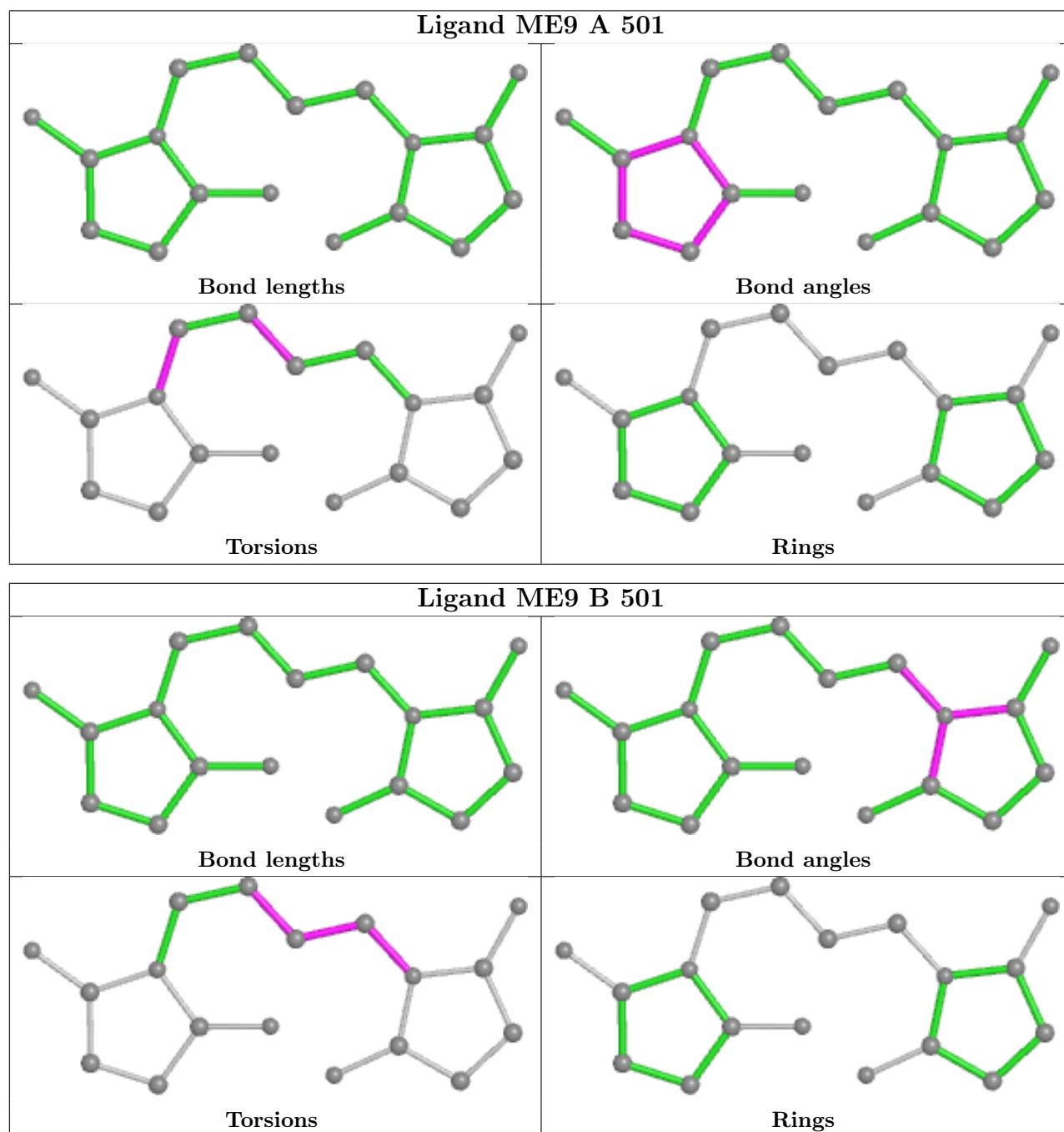
There are no ring outliers.

1 monomer is involved in 1 short contact:

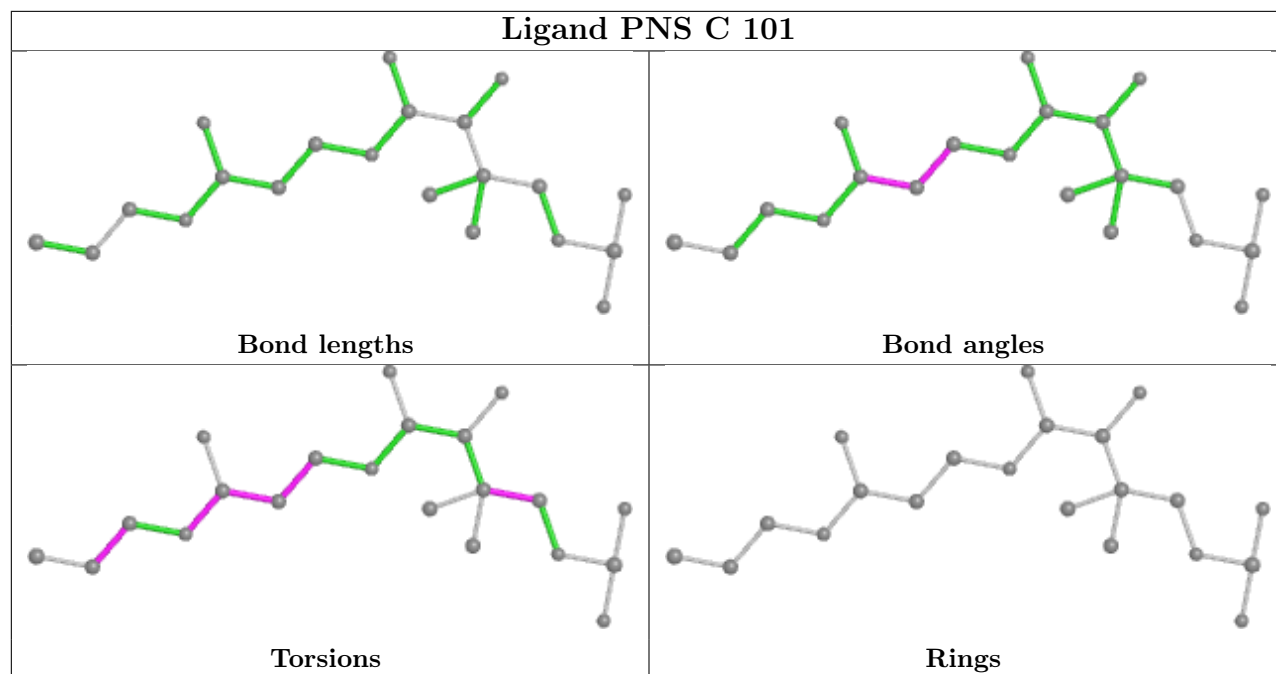
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	ME9	1	0

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	444/466 (95%)	-0.16	6 (1%) 75 71	23, 36, 74, 117	0
1	B	444/466 (95%)	-0.24	9 (2%) 65 60	24, 37, 63, 124	0
2	C	86/107 (80%)	1.78	38 (44%) 0 0	42, 77, 120, 156	0
All	All	974/1039 (93%)	-0.02	53 (5%) 25 20	23, 38, 89, 156	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	28	HIS	5.5
2	C	34	ILE	5.4
2	C	38	ARG	4.9
2	C	35	GLU	4.8
2	C	23	ALA	4.3
2	C	37	GLY	4.2
2	C	32	GLU	4.0
1	A	444	GLN	4.0
2	C	43	LEU	3.9
2	C	87	VAL	3.8
2	C	31	GLY	3.7
2	C	30	SER	3.5
2	C	68	THR	3.5
1	A	442	ALA	3.5
1	B	249	ASP	3.4
2	C	39	ALA	3.3
2	C	42	ASN	3.3
2	C	33	ASP	3.3
1	B	250	ALA	3.2
2	C	62	GLY	3.2
1	B	83	PRO	3.2
2	C	14	LEU	3.0
2	C	74	PRO	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	71	PHE	3.0
1	A	250	ALA	3.0
1	B	247	ASN	2.9
2	C	61	THR	2.9
2	C	75	ASN	2.9
2	C	40	PHE	2.9
2	C	22	VAL	2.9
2	C	45	PHE	2.9
1	A	245	ARG	2.9
1	A	441	TYR	2.8
1	B	246	PHE	2.8
2	C	44	GLY	2.8
1	B	248	GLY	2.8
2	C	69	ILE	2.7
2	C	82	HIS	2.7
2	C	81	GLN	2.6
1	B	80	GLU	2.6
2	C	36	PRO	2.6
2	C	27	GLY	2.6
2	C	86	ALA	2.6
2	C	85	ALA	2.5
2	C	41	LYS	2.5
1	B	251	GLU	2.5
2	C	29	ALA	2.4
2	C	24	ALA	2.3
2	C	59	ALA	2.2
1	B	69	GLU	2.2
1	A	287	ALA	2.1
2	C	21	GLN	2.0
2	C	78	ALA	2.0

## 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](#)

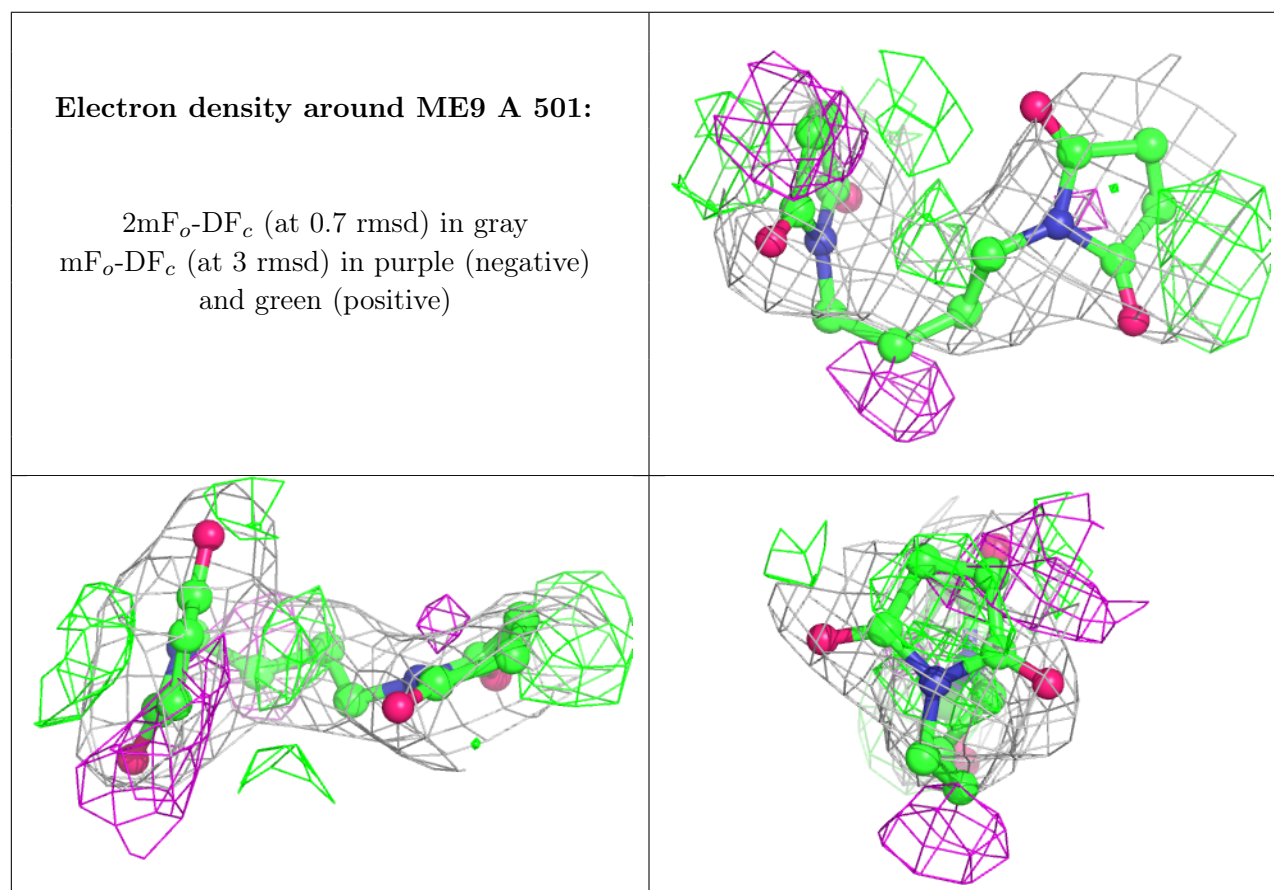
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

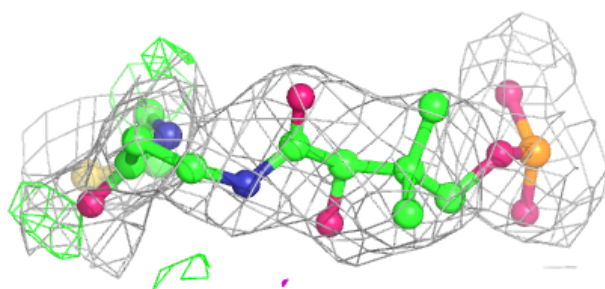
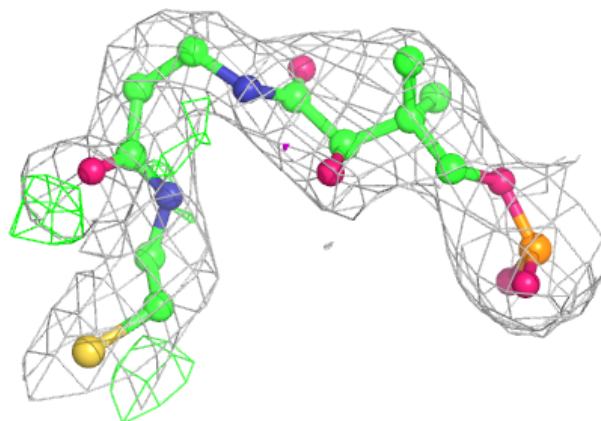
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ME9	A	501	18/18	0.81	0.28	50,62,69,72	0
4	PNS	C	101	21/22	0.89	0.18	47,54,81,93	0
3	ME9	B	501	18/18	0.91	0.17	44,55,67,68	0

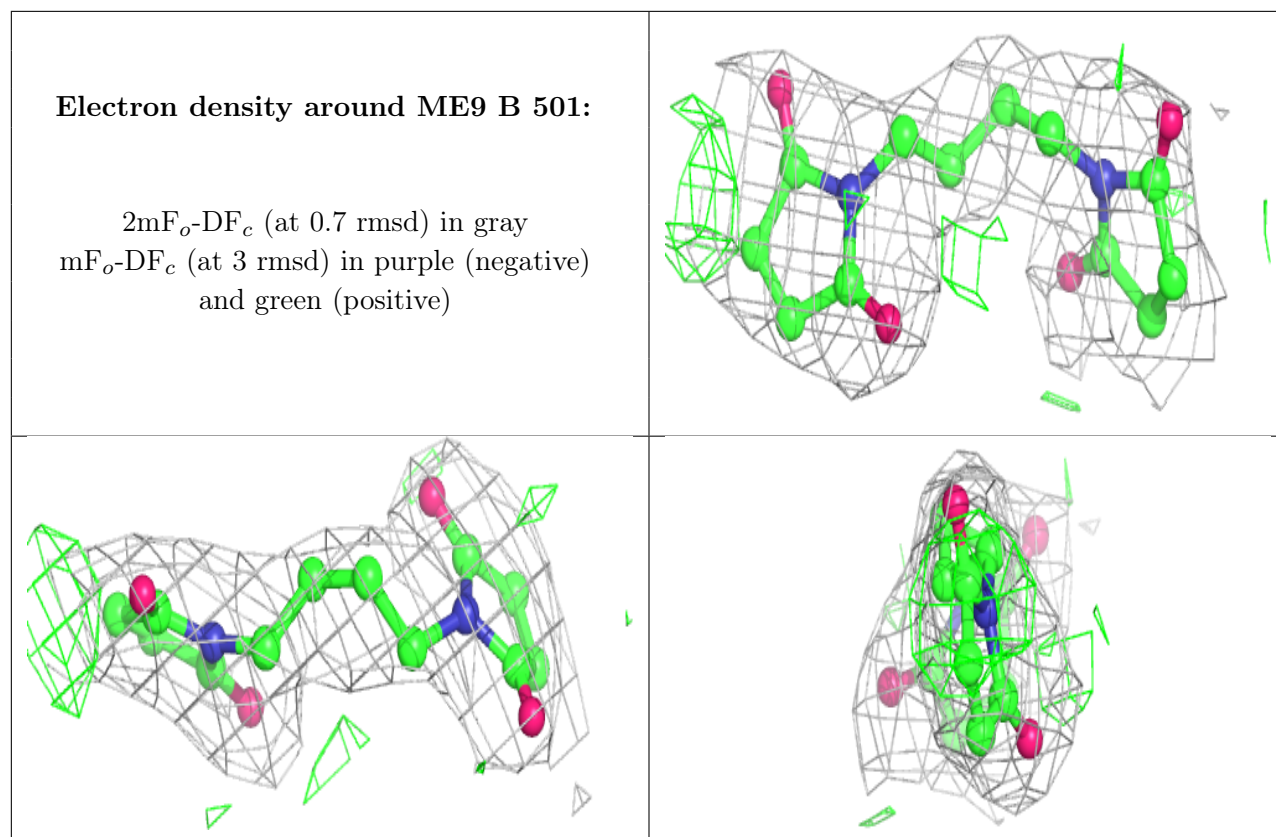
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around PNS C 101:**

$2mF_o-DF_c$  (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.