Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2026 – 07:28 am BST

PDB ID	:	8C3B / pdb_00008c3b
Title	:	X-ray structure of RNase A upon reaction with a Ruthenium(II)-arene Complexed with Glycosylated Carbene Ligands (5)
Authors	:	Ferraro, G.; Merlino, A.
Deposited on	:	2022-12-23
Resolution	:	1.24 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

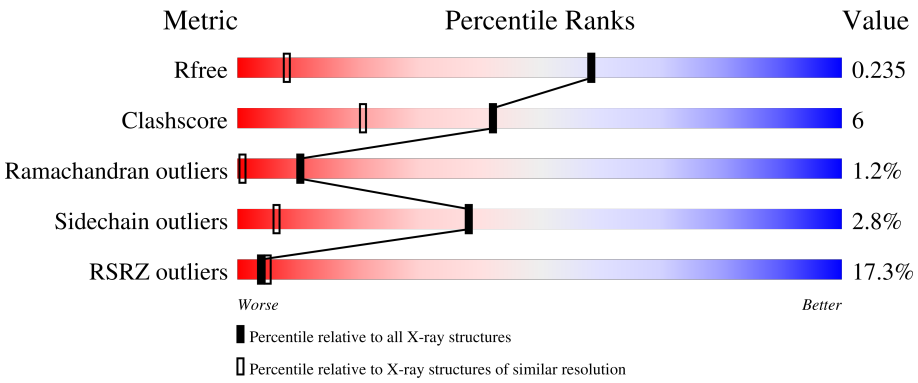
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.24 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}	180053	1630 (1.26-1.22)
Clashscore	190562	1668 (1.26-1.22)
Ramachandran outliers	187476	1635 (1.26-1.22)
Sidechain outliers	187428	1633 (1.26-1.22)
RSRZ outliers	180081	1630 (1.26-1.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	AAA	124	15% 88% 10% • •
1	BBB	124	20% 90% 9% •

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
3	T9L	AAA	202	-	-	X	-

2 Entry composition (i)

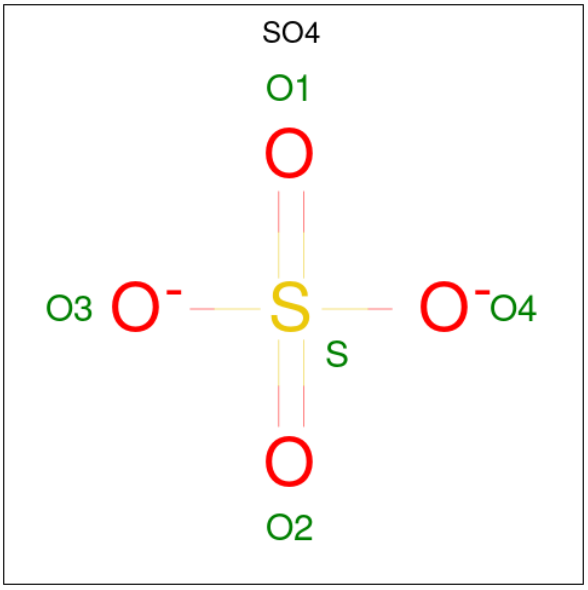
There are 4 unique types of molecules in this entry. The entry contains 2369 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribonuclease pancreatic.

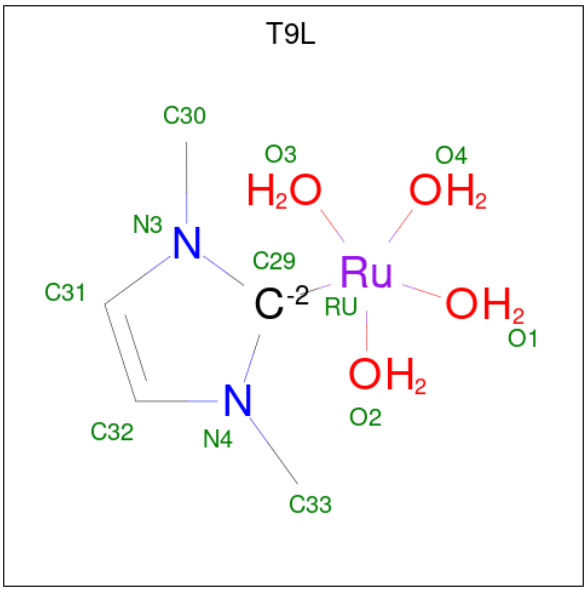
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	124	989	595	178	204	12	0	5	0
1	BBB	124	1017	613	183	208	13	0	8	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	AAA	1	5	4	1	0	0

- Molecule 3 is (1,3-dimethylimidazol-2-yl)-tetrakis($l^{3}-oxidanyl)ruthenium (CCD ID: T9L) (formula: $C_5H_{16}N_2O_4Ru$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	Ru	0	0
			11	5	2	3	1		
3	BBB	1	Total	C	N	O	Ru	0	1
			12	5	2	4	1		
3	BBB	1	Total	C	N	O	Ru	0	0
			10	5	2	2	1		

- Molecule 4 is water.

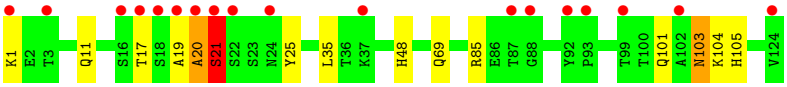
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	162	Total	O	0	4
			164	164		
4	BBB	160	Total	O	0	6
			161	161		

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.

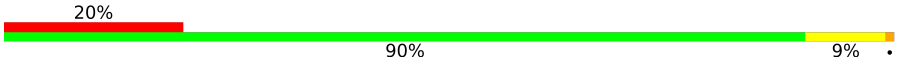
- Molecule 1: Ribonuclease pancreatic

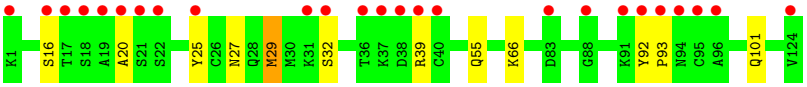
Chain AAA:



- Molecule 1: Ribonuclease pancreatic

Chain BBB:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	100.74Å 32.92Å 72.63Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	72.63 – 1.24 72.63 – 1.24	Depositor EDS
% Data completeness (in resolution range)	88.0 (72.63-1.24) 88.0 (72.63-1.24)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 1.24Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.192 , 0.227 0.200 , 0.235	Depositor DCC
R_{free} test set	2940 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2369	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, T9L

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	AAA	1.11	0/1005	1.23	1/1355 (0.1%)
1	BBB	1.09	0/1033	1.14	2/1390 (0.1%)
All	All	1.10	0/2038	1.19	3/2745 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	27	ASN	CA-C-N	5.26	127.60	120.44
1	BBB	27	ASN	C-N-CA	5.26	127.60	120.44
1	AAA	103	ASN	CA-CB-CG	-5.05	107.55	112.60

There are no chirality outliers.

There are no planarity outliers.

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	AAA	989	0	930	12	0
1	BBB	1017	0	961	7	0
2	AAA	5	0	0	0	0
3	AAA	11	0	0	7	0
3	BBB	22	0	0	0	0
4	AAA	164	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	161	0	0	1	0
All	All	2369	0	1891	25	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 6.

All (25) 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)
3:AAA:202:T9L:O2	3:AAA:202:T9L:RU	1.24	0.97
3:AAA:202:T9L:O2	3:AAA:202:T9L:C29	2.28	0.81
3:AAA:202:T9L:C33	4:AAA:349[B]:HOH:O	2.33	0.77
1:BBB:20:ALA:HB3	1:BBB:101:GLN:OE1	1.86	0.75
1:AAA:105:HIS:NE2	3:AAA:202:T9L:O2	2.20	0.74
1:AAA:101:GLN:HG3	4:AAA:315:HOH:O	1.87	0.72
1:AAA:20:ALA:HB2	1:AAA:101:GLN:HB2	1.74	0.68
3:AAA:202:T9L:O2	3:AAA:202:T9L:C30	2.44	0.65
1:AAA:20:ALA:O	1:AAA:21:SER:HB3	2.00	0.59
3:AAA:202:T9L:O2	3:AAA:202:T9L:O3	2.23	0.56
1:AAA:11:GLN:HG2	1:AAA:35:LEU:HD21	1.91	0.53
1:AAA:19:ALA:O	1:AAA:20:ALA:C	2.52	0.52
3:AAA:202:T9L:O2	3:AAA:202:T9L:N3	2.45	0.50
1:AAA:69[A]:GLN:NE2	4:AAA:302:HOH:O	2.26	0.49
1:BBB:55:GLN:HB3	4:BBB:307:HOH:O	2.14	0.48
1:AAA:17:THR:O	1:AAA:48:HIS:HB3	2.16	0.46
1:BBB:20:ALA:HB1	1:BBB:25:TYR:CG	2.50	0.45
1:BBB:66[B]:LYS:HE2	1:BBB:66[B]:LYS:C	2.41	0.45
1:AAA:104:LYS:NZ	4:AAA:313:HOH:O	2.50	0.45
1:AAA:20:ALA:N	1:AAA:101:GLN:NE2	2.65	0.44
1:BBB:29[B]:MET:HE3	1:BBB:29[B]:MET:HB3	1.79	0.43
1:AAA:103:ASN:ND2	4:AAA:315:HOH:O	2.52	0.43
1:BBB:25:TYR:CZ	1:BBB:29[A]:MET:HG3	2.56	0.41
1:BBB:92:TYR:CD1	1:BBB:93:PRO:HA	2.55	0.41
1:AAA:21:SER:HB3	1:AAA:25:TYR:CD1	2.56	0.40

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
1	AAA	127/124 (102%)	120 (94%)	5 (4%)	2 (2%)	7 0
1	BBB	130/124 (105%)	120 (92%)	9 (7%)	1 (1%)	16 3
All	All	257/248 (104%)	240 (93%)	14 (5%)	3 (1%)	10 1

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	21	SER
1	AAA	20	ALA
1	BBB	16	SER

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	AAA	114/109 (105%)	111 (97%)	3 (3%)	40 7
1	BBB	117/109 (107%)	113 (97%)	4 (3%)	32 4
All	All	231/218 (106%)	224 (97%)	7 (3%)	38 5

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	1	LYS
1	AAA	21	SER
1	AAA	85	ARG

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Mol	Chain	Res	Type
1	BBB	29[A]	MET
1	BBB	29[B]	MET
1	BBB	32	SER
1	BBB	39	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	T9L	BBB	202	1	5,10,12	5.50	3 (60%)	6,14,21	2.58	4 (66%)
3	T9L	AAA	202	1	5,11,12	5.41	3 (60%)	6,17,21	2.82	4 (66%)
2	SO4	AAA	201	-	4,4,4	0.49	0	6,6,6	0.20	0
3	T9L	BBB	201[A]	1	5,12,12	5.56	3 (60%)	6,21,21	2.15	2 (33%)

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	T9L	BBB	202	1	-	-	0/1/1/1
3	T9L	AAA	202	1	-	-	0/1/1/1
3	T9L	BBB	201[A]	1	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	201[A]	T9L	C33-N4	-9.14	1.32	1.46
3	AAA	202	T9L	C33-N4	-9.13	1.32	1.46
3	BBB	202	T9L	C33-N4	-9.11	1.32	1.46
3	BBB	201[A]	T9L	C30-N3	-7.93	1.34	1.46
3	BBB	202	T9L	C30-N3	-7.75	1.34	1.46
3	AAA	202	T9L	C30-N3	-7.43	1.35	1.46
3	BBB	202	T9L	C32-N4	-2.51	1.33	1.38
3	BBB	201[A]	T9L	C32-N4	-2.48	1.33	1.38
3	AAA	202	T9L	C32-N4	-2.40	1.33	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	202	T9L	C30-N3-C31	-4.38	114.98	123.56
3	BBB	201[A]	T9L	C29-N3-C31	-3.97	100.65	109.48
3	BBB	202	T9L	C33-N4-C32	-3.68	116.35	123.56
3	AAA	202	T9L	C30-N3-C29	3.59	138.36	120.15
3	BBB	202	T9L	C33-N4-C29	3.16	136.18	120.15
3	BBB	202	T9L	C29-N3-C31	-3.01	102.78	109.48
3	AAA	202	T9L	C33-N4-C32	-2.96	117.76	123.56
3	BBB	201[A]	T9L	C30-N3-C29	2.75	134.09	120.15
3	BBB	202	T9L	C30-N3-C29	2.51	132.88	120.15
3	AAA	202	T9L	C33-N4-C29	2.00	130.29	120.15

There are no chirality outliers.

There are no torsion outliers.

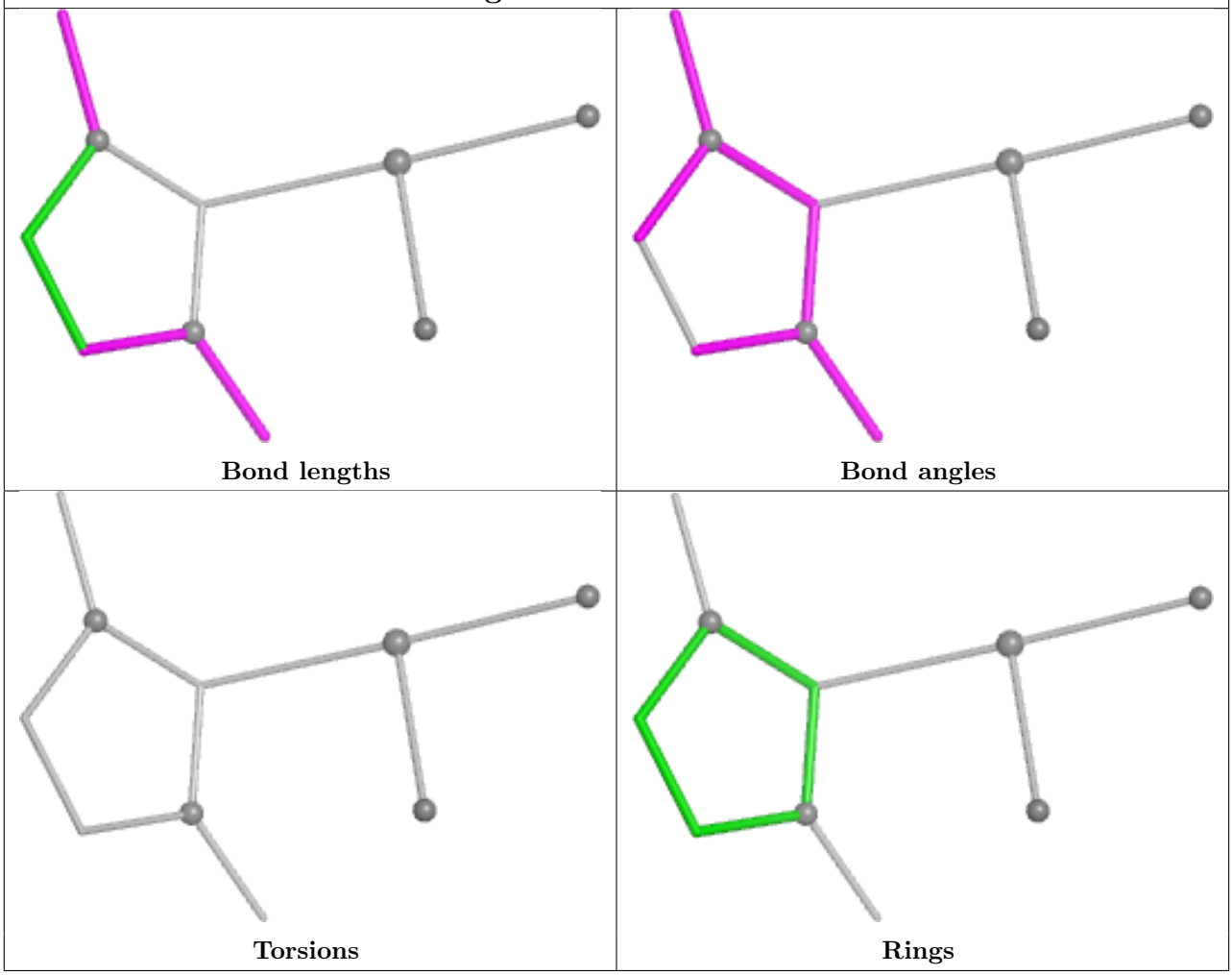
There are no ring outliers.

1 monomer is involved in 7 short contacts:

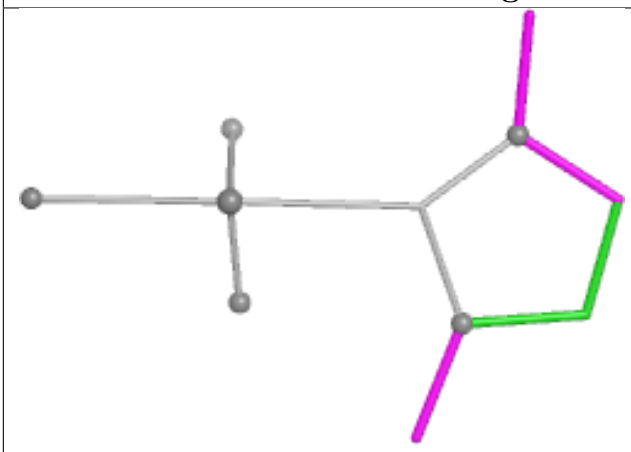
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	202	T9L	7	0

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 then 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.

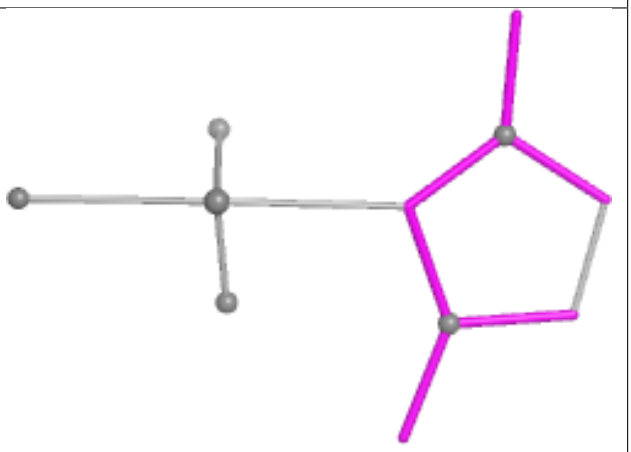
Ligand T9L BBB 202



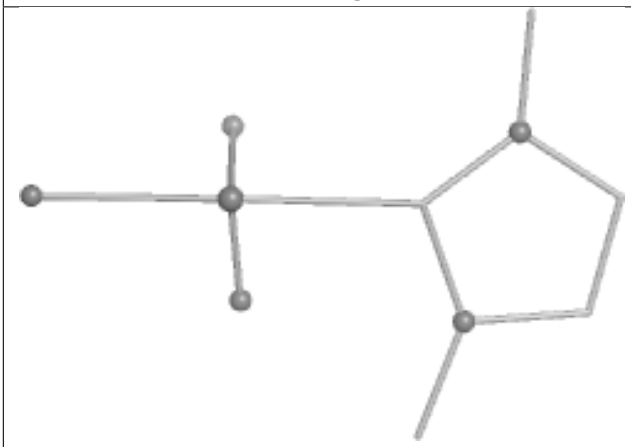
Ligand T9L AAA 202



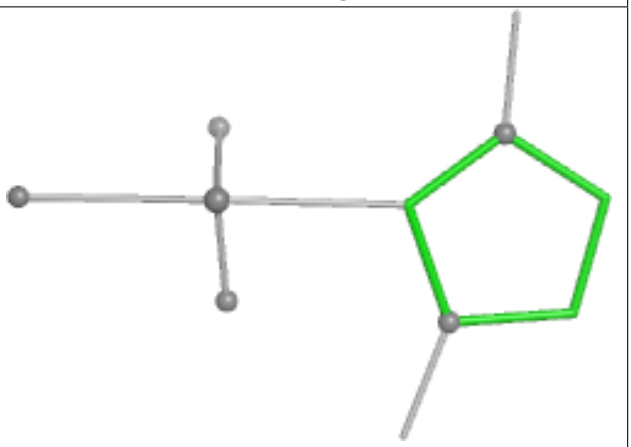
Bond lengths



Bond angles

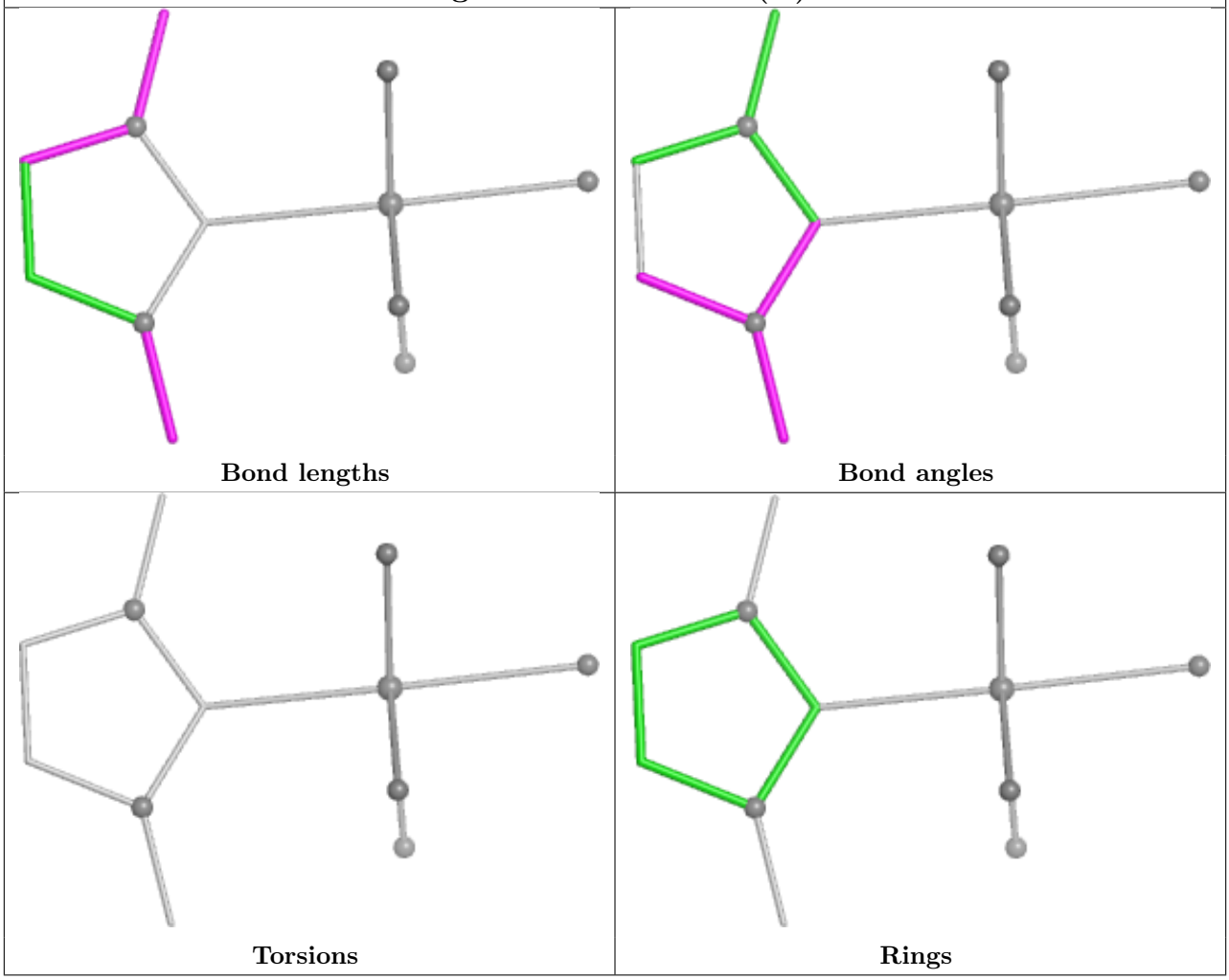


Torsions



Rings

Ligand T9L BBB 201 (A)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	124/124 (100%)	1.00	18 (14%)	6	6	8, 24, 55, 69	5 (4%)
1	BBB	124/124 (100%)	1.13	25 (20%)	3	3	9, 22, 56, 104	8 (6%)
All	All	248/248 (100%)	1.06	43 (17%)	4	5	8, 23, 56, 104	13 (5%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	19	ALA	10.0
1	AAA	21	SER	7.4
1	BBB	20	ALA	6.9
1	BBB	18	SER	5.6
1	AAA	20	ALA	5.4
1	BBB	16	SER	5.3
1	AAA	88	GLY	4.7
1	BBB	17	THR	4.3
1	AAA	17	THR	4.0
1	AAA	92	TYR	3.9
1	BBB	21	SER	3.7
1	AAA	19	ALA	3.5
1	AAA	18	SER	3.4
1	BBB	92	TYR	3.3
1	BBB	94[A]	ASN	3.3
1	BBB	25	TYR	3.2
1	BBB	39	ARG	3.1
1	BBB	88	GLY	3.0
1	BBB	22	SER	2.9
1	AAA	93	PRO	2.9
1	AAA	87	THR	2.9
1	BBB	38	ASP	2.8
1	BBB	96	ALA	2.8
1	BBB	95	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	AAA	24[A]	ASN	2.7
1	BBB	36	THR	2.7
1	AAA	22	SER	2.6
1	AAA	16	SER	2.5
1	BBB	83	ASP	2.5
1	AAA	124	VAL	2.5
1	BBB	91	LYS	2.5
1	BBB	32	SER	2.4
1	AAA	99	THR	2.3
1	AAA	1	LYS	2.3
1	AAA	3	THR	2.2
1	BBB	93	PRO	2.2
1	BBB	1	LYS	2.2
1	AAA	102	ALA	2.2
1	BBB	124	VAL	2.2
1	AAA	37	LYS	2.2
1	BBB	37	LYS	2.1
1	BBB	40	CYS	2.1
1	BBB	31	LYS	2.1

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 oligosaccharides in this entry.

6.4 Ligands (i)

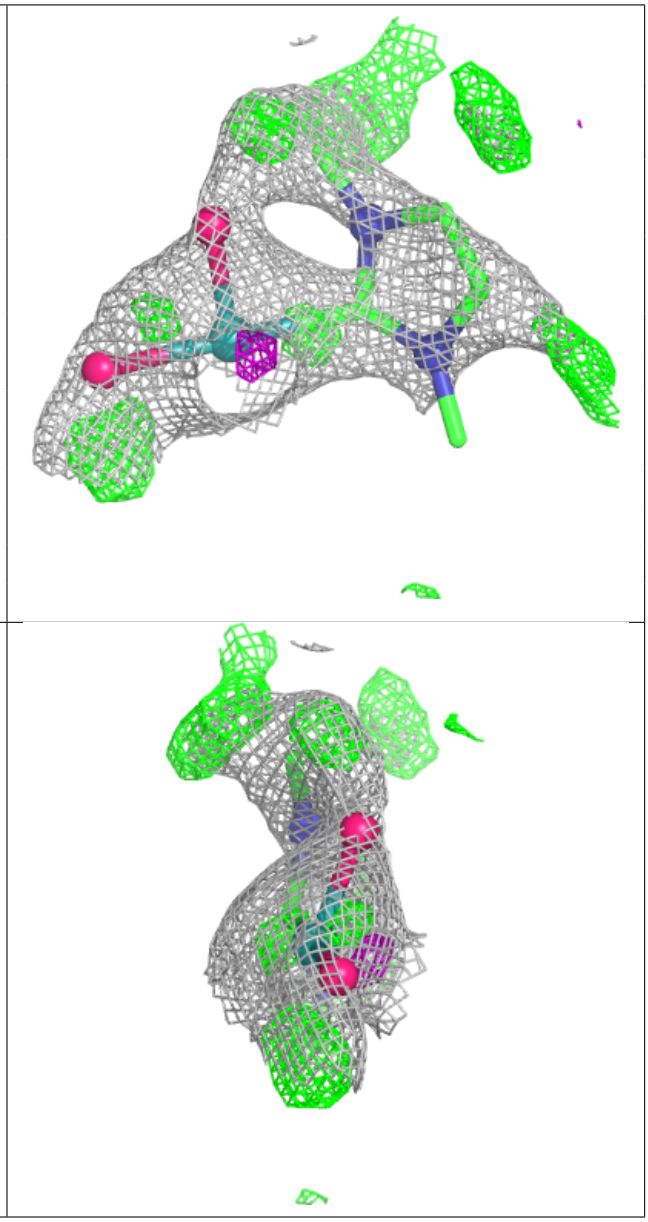
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	AAA	201	5/5	0.94	0.10	23,24,30,34	5
3	T9L	BBB	202	10/12	0.94	0.18	33,42,44,45	10
3	T9L	AAA	202	11/12	0.95	0.16	14,28,32,35	11
3	T9L	BBB	201[A]	12/12	0.97	0.15	20,21,24,24	12

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.

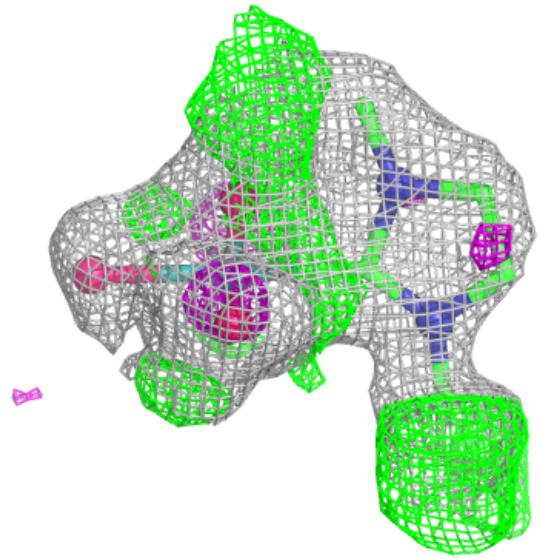
Electron density around T9L BBB 202:

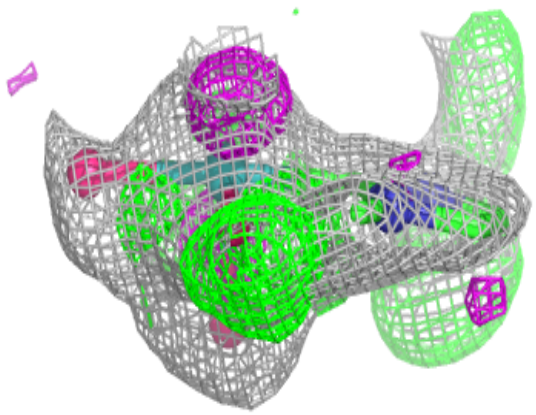
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

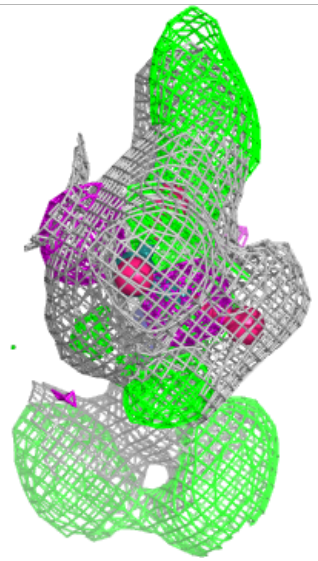


Electron density around T9L AAA 202:

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

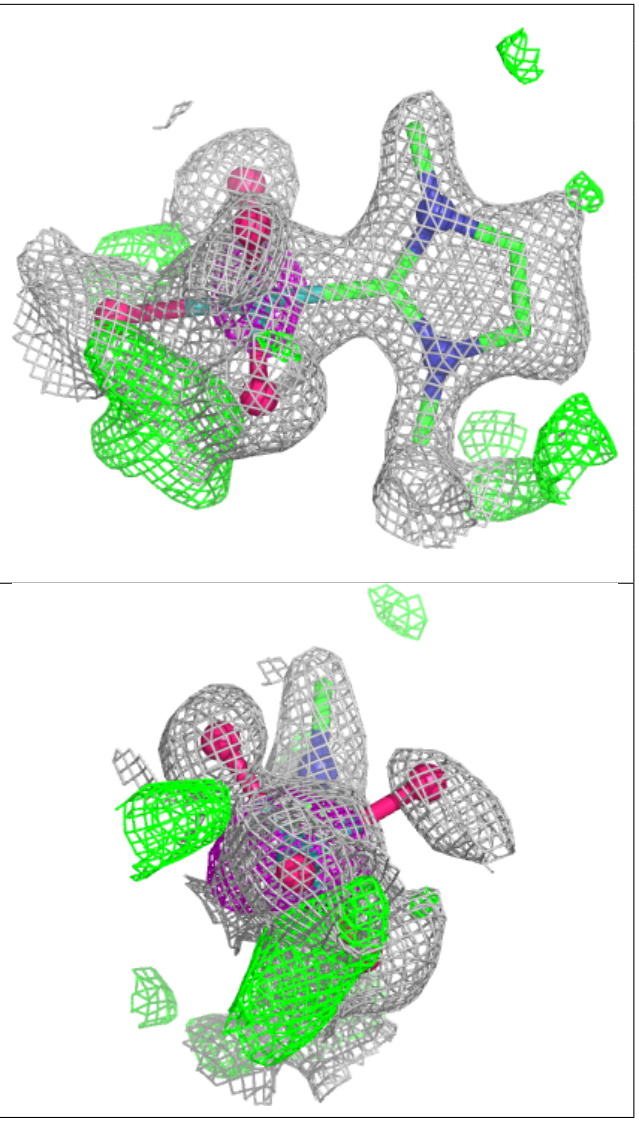






Electron density around T9L BBB 201 (A):

$2mF_o$-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.