



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 11:47 AM BST

PDB ID : 6M13
Title : Crystal structure of Rnase L in complex with Toceranib
Authors : Tang, J.; Huang, H.
Deposited on : 2020-02-24
Resolution : 2.56 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 ⓘ 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 : 2.13
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) : 2.13

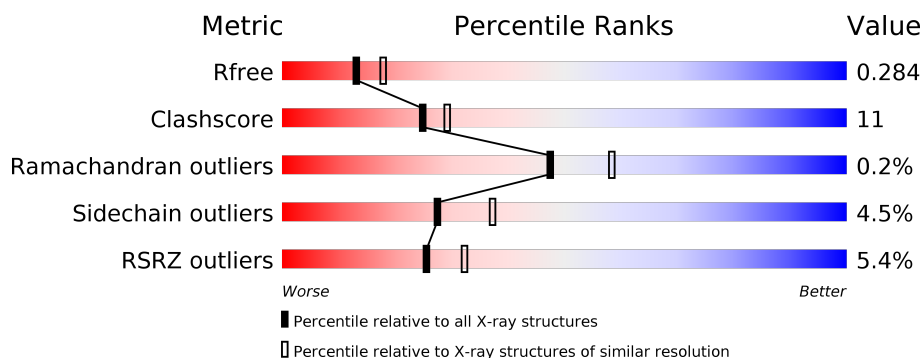
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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 on 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 $\leq 5\%$. 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	717	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	b	717	<div> <div>7%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11078 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.

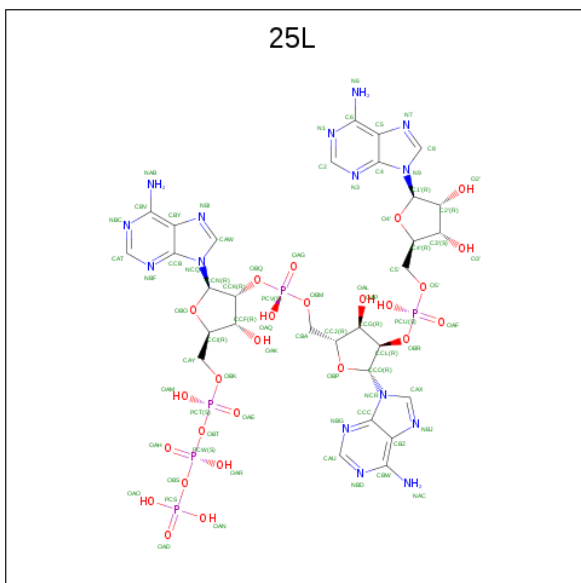
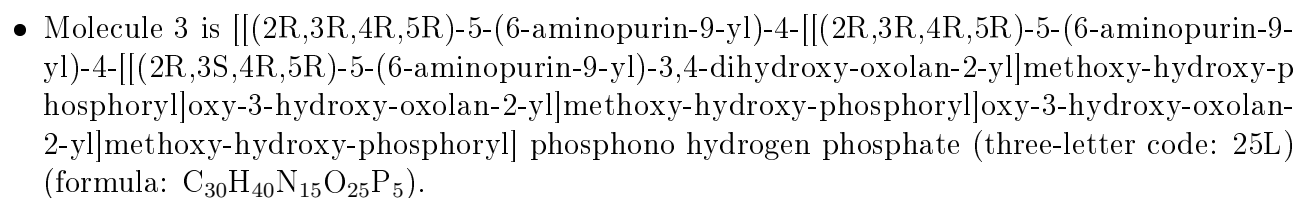
- Molecule 1 is a protein called Ribonuclease L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	681	Total	C	N	O	S	0	0	0
			5408	3395	953	1038	22			
1	b	688	Total	C	N	O	S	0	0	0
			5463	3425	968	1049	21			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	16	GLY	-	expression tag	UNP A5H025
a	17	ALA	-	expression tag	UNP A5H025
a	18	MET	-	expression tag	UNP A5H025
a	19	ASP	-	expression tag	UNP A5H025
a	20	PRO	-	expression tag	UNP A5H025
b	16	GLY	-	expression tag	UNP A5H025
b	17	ALA	-	expression tag	UNP A5H025
b	18	MET	-	expression tag	UNP A5H025
b	19	ASP	-	expression tag	UNP A5H025
b	20	PRO	-	expression tag	UNP A5H025

- Molecule 2 is 5-[(Z)-(5-fluoranyl-2-oxidanylidene-1H-indol-3-ylidene)methyl]-2,4-dimethyl-N-(2-pyrrolidin-1-ylethyl)-1H-pyrrole-3-carboxamide (three-letter code: BWC) (formula: C₂₂H₂₅FN₄O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	a	1	Total	C	N	O	P	0	0
			67	30	15	19	3		
3	b	1	Total	C	N	O	P	0	0
			67	30	15	19	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	a	1	Total	O	P	0	0
			5	4	1		

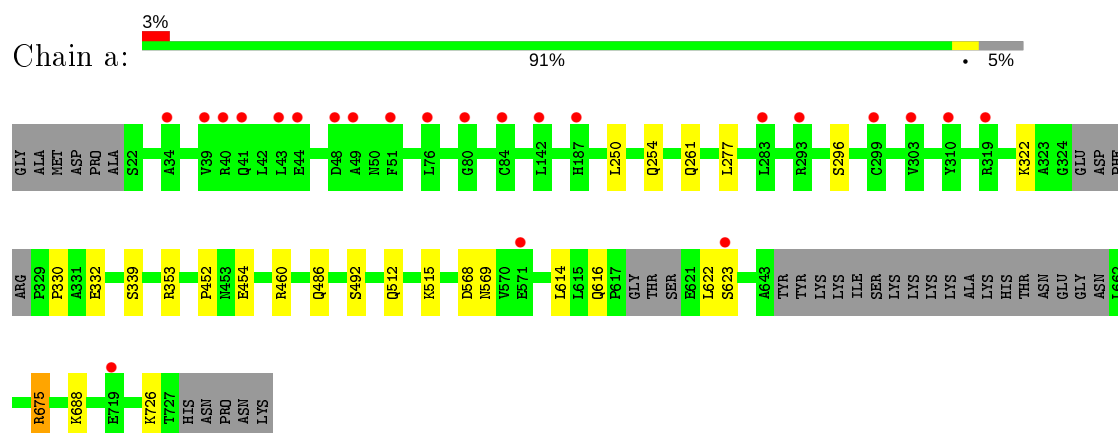
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	a	7	Total	O	0	0
			7	7		
5	b	3	Total	O	0	0
			3	3		

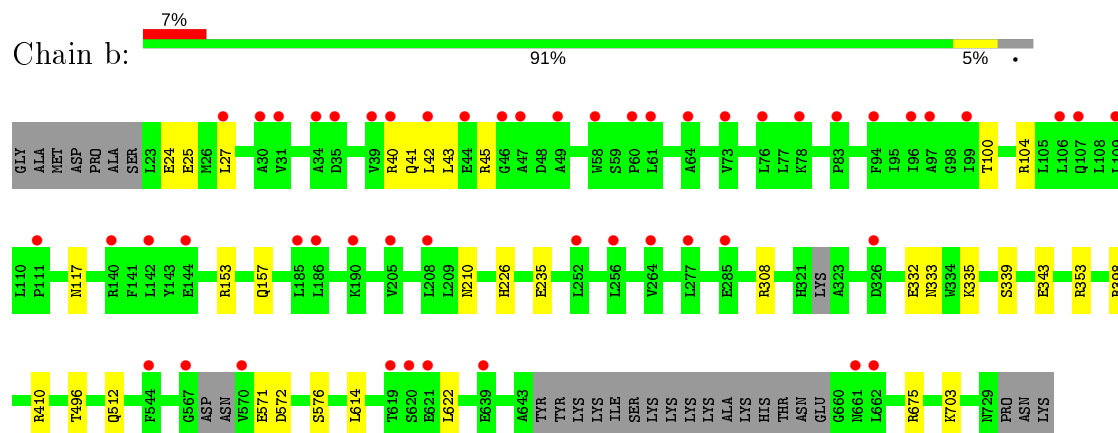
3 Residue-property plots

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: Ribonuclease L



• Molecule 1: Ribonuclease L



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.45Å 111.36Å 263.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.02 – 2.56 69.02 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.3 (69.02-2.56) 99.3 (69.02-2.56)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.231 , 0.286 0.232 , 0.284	Depositor DCC
R_{free} test set	2883 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11078	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PO4, BWC, 25L

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	0.58	0/5503	0.74	3/7430 (0.0%)
1	b	0.57	0/5560	0.76	3/7508 (0.0%)
All	All	0.57	0/11063	0.75	6/14938 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	353	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	b	410	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	a	675	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	b	353	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	b	153	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	a	460	ARG	NE-CZ-NH2	-5.14	117.73	120.30

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	a	5408	0	5325	0	0
1	b	5463	0	5360	0	0
2	a	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	29	0	0	0	0
3	a	67	0	31	0	0
3	b	67	0	31	0	0
4	a	5	0	0	0	0
5	a	7	0	0	0	0
5	b	3	0	0	0	0
All	All	11078	0	10747	0	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 11.

There are no clashes within the asymmetric unit.

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	a	673/717 (94%)	643 (96%)	28 (4%)	2 (0%)	41	50
1	b	680/717 (95%)	649 (95%)	30 (4%)	1 (0%)	51	65
All	All	1353/1434 (94%)	1292 (96%)	58 (4%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	623	SER
1	b	332	GLU
1	a	330	PRO

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	582/617 (94%)	560 (96%)	22 (4%)	33	44
1	b	586/617 (95%)	556 (95%)	30 (5%)	24	32
All	All	1168/1234 (95%)	1116 (96%)	52 (4%)	27	37

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	250	LEU
1	a	254	GLN
1	a	261	GLN
1	a	277	LEU
1	a	296	SER
1	a	322	LYS
1	a	332	GLU
1	a	339	SER
1	a	452	PRO
1	a	454	GLU
1	a	486	GLN
1	a	492	SER
1	a	512	GLN
1	a	515	LYS
1	a	568	ASP
1	a	569	ASN
1	a	614	LEU
1	a	616	GLN
1	a	622	LEU
1	a	675	ARG
1	a	688	LYS
1	a	726	LYS
1	b	24	GLU
1	b	25	GLU
1	b	27	LEU
1	b	40	ARG
1	b	41	GLN
1	b	42	LEU
1	b	43	LEU
1	b	45	ARG
1	b	100	THR

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Mol	Chain	Res	Type
1	b	104	ARG
1	b	117	ASN
1	b	157	GLN
1	b	210	ASN
1	b	226	HIS
1	b	235	GLU
1	b	308	ARG
1	b	333	ASN
1	b	335	LYS
1	b	339	SER
1	b	343	GLU
1	b	398	ARG
1	b	496	THR
1	b	512	GLN
1	b	571	GLU
1	b	572	ASP
1	b	576	SER
1	b	614	LEU
1	b	622	LEU
1	b	675	ARG
1	b	703	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	41	GLN
1	a	50	ASN
1	a	249	ASN
1	a	400	GLN
1	a	407	GLN
1	a	569	ASN
1	a	608	ASN
1	a	698	GLN
1	b	52	GLN
1	b	79	HIS
1	b	107	GLN
1	b	112	ASN
1	b	152	HIS
1	b	210	ASN
1	b	226	HIS
1	b	333	ASN
1	b	453	ASN

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Mol	Chain	Res	Type
1	b	616	GLN
1	b	716	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	25L	a	802	-	64,75,83	4.35	23 (35%)	75,116,130	2.28	14 (18%)
2	BWC	b	901	-	28,32,32	2.76	9 (32%)	34,46,46	2.04	9 (26%)
4	PO4	a	803	-	4,4,4	0.96	0	6,6,6	0.93	1 (16%)
2	BWC	a	801	-	28,32,32	2.65	8 (28%)	34,46,46	2.20	12 (35%)
3	25L	b	902	-	64,75,83	4.33	24 (37%)	75,116,130	2.22	15 (20%)

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	25L	a	802	-	-	3/28/88/100	0/9/9/9
2	BWC	b	901	-	-	1/10/33/33	0/4/4/4
2	BWC	a	801	-	-	3/10/33/33	0/4/4/4
3	25L	b	902	-	-	12/28/88/100	0/9/9/9

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	902	25L	O4'-C1'	17.08	1.64	1.41
3	a	802	25L	O4'-C1'	16.30	1.63	1.41
3	a	802	25L	OBO-CCN	15.95	1.63	1.41
3	b	902	25L	OBP-CCO	15.01	1.62	1.41
3	a	802	25L	OBP-CCO	14.93	1.61	1.41
3	b	902	25L	OBO-CCN	14.79	1.61	1.41
3	a	802	25L	C2'-C1'	-13.40	1.33	1.53
3	b	902	25L	C2'-C1'	-12.04	1.35	1.53
2	b	901	BWC	CAJ-CAI	-8.15	1.38	1.50
2	a	801	BWC	CAP-CAT	-7.25	1.40	1.51
2	a	801	BWC	CAJ-CAI	-7.24	1.39	1.50
2	b	901	BWC	CAP-CAT	-6.98	1.40	1.51
3	b	902	25L	OBO-CCI	-6.74	1.29	1.45
3	b	902	25L	O4'-C4'	-6.14	1.31	1.45
3	a	802	25L	OBP-CCJ	-6.05	1.31	1.45
3	a	802	25L	O4'-C4'	-5.40	1.32	1.45
3	a	802	25L	OBO-CCI	-5.36	1.33	1.45
3	b	902	25L	OBP-CCJ	-4.95	1.33	1.45
2	b	901	BWC	CAS-CAO	4.48	1.58	1.50
3	a	802	25L	OAL-CCG	-4.38	1.32	1.43
2	b	901	BWC	CAL-CAJ	4.30	1.41	1.34
3	b	902	25L	OAL-CCG	-4.23	1.33	1.43
2	a	801	BWC	CAE-CAJ	-4.09	1.38	1.45
3	a	802	25L	C6-N6	4.02	1.48	1.34
3	a	802	25L	CBW-NAC	3.98	1.48	1.34
3	b	902	25L	C6-N6	3.96	1.48	1.34
3	b	902	25L	C2-N3	3.95	1.38	1.32
2	a	801	BWC	CAL-CAJ	3.87	1.40	1.34
3	b	902	25L	CBW-NAC	3.86	1.48	1.34
2	a	801	BWC	CAS-CAO	3.84	1.56	1.50
2	b	901	BWC	CAE-CAJ	-3.75	1.39	1.45
3	a	802	25L	PCT-OBT	3.72	1.69	1.54
3	a	802	25L	C2-N3	3.68	1.38	1.32
3	b	902	25L	OAK-CCF	-3.66	1.34	1.43
3	b	902	25L	O3'-C3'	-3.62	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	802	25L	O3'-C3'	-3.45	1.34	1.43
3	b	902	25L	CAU-NBG	3.29	1.37	1.32
3	b	902	25L	PCT-OBT	3.27	1.67	1.54
3	b	902	25L	CBY-CCB	-3.09	1.32	1.40
3	a	802	25L	CCF-CCI	3.01	1.60	1.53
2	a	801	BWC	CAT-NAV	2.85	1.40	1.33
3	a	802	25L	OAK-CCF	-2.81	1.36	1.43
3	b	902	25L	CBZ-CCC	-2.75	1.33	1.40
3	b	902	25L	CAT-NBF	2.75	1.36	1.32
3	b	902	25L	O2'-C2'	2.72	1.49	1.43
3	a	802	25L	CBZ-CCC	-2.65	1.33	1.40
3	a	802	25L	CAT-NBF	2.62	1.36	1.32
3	b	902	25L	PCU-O5'	2.62	1.69	1.59
3	b	902	25L	PCV-OBQ	2.58	1.67	1.60
2	b	901	BWC	CAE-CAD	-2.55	1.38	1.41
2	a	801	BWC	CAR-CAQ	2.50	1.56	1.51
3	a	802	25L	CBY-CCB	-2.49	1.34	1.40
3	a	802	25L	C5-C4	-2.48	1.34	1.40
3	b	902	25L	CBV-NAB	2.44	1.42	1.34
2	a	801	BWC	CAC-CAD	-2.43	1.35	1.39
2	b	901	BWC	CAT-NAV	2.40	1.39	1.33
3	a	802	25L	O2'-C2'	2.38	1.48	1.43
3	b	902	25L	C5-C4	-2.37	1.34	1.40
3	a	802	25L	CBV-NAB	2.34	1.42	1.34
2	b	901	BWC	CAR-CAQ	2.09	1.56	1.51
3	a	802	25L	CCG-CCJ	2.03	1.58	1.53
2	b	901	BWC	CAC-CAD	-2.03	1.36	1.39
3	a	802	25L	PCU-O5'	2.02	1.67	1.59
3	b	902	25L	CCG-CCJ	2.00	1.58	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	802	25L	CBZ-CBW-NAC	8.53	133.32	120.35
3	b	902	25L	CBZ-CBW-NAC	7.35	131.53	120.35
3	b	902	25L	CBY-CBV-NAB	7.31	131.46	120.35
3	a	802	25L	CBY-CBV-NAB	7.05	131.07	120.35
3	a	802	25L	N3-C2-N1	-5.82	119.58	128.68
2	b	901	BWC	CAX-NAY-CBC	-5.64	97.62	113.29
3	b	902	25L	NBG-CAU-NBD	-5.53	120.03	128.68
3	a	802	25L	NAC-CBW-NBD	-5.52	107.12	118.57
3	b	902	25L	C3'-C2'-C1'	5.45	109.18	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	902	25L	N3-C2-N1	-5.41	120.23	128.68
3	a	802	25L	C3'-C2'-C1'	5.34	109.02	100.98
3	a	802	25L	NBG-CAU-NBD	-5.20	120.54	128.68
3	b	902	25L	NBF-CAT-NBC	-5.19	120.57	128.68
2	a	801	BWC	CAD-NAH-CAI	-5.17	108.13	111.38
3	b	902	25L	NAC-CBW-NBD	-5.16	107.86	118.57
3	a	802	25L	NBF-CAT-NBC	-5.05	120.78	128.68
3	b	902	25L	NAB-CBV-NBC	-4.73	108.75	118.57
3	a	802	25L	C5-C6-N6	4.65	127.42	120.35
2	b	901	BWC	CAJ-CAI-NAH	4.42	109.36	106.88
2	a	801	BWC	CAX-NAY-CBC	-4.34	101.23	113.29
2	a	801	BWC	CAJ-CAI-NAH	4.10	109.18	106.88
3	a	802	25L	NAB-CBV-NBC	-4.00	110.27	118.57
2	b	901	BWC	CAD-NAH-CAI	-3.93	108.91	111.38
2	a	801	BWC	CAX-NAY-CAZ	3.90	124.12	113.29
2	a	801	BWC	CAB-CAA-CAF	-3.46	118.80	123.29
3	b	902	25L	C5-C6-N6	3.37	125.47	120.35
2	a	801	BWC	CAL-CAJ-CAI	3.33	133.37	119.96
2	b	901	BWC	CAB-CAA-CAF	-3.28	119.03	123.29
3	a	802	25L	OBQ-CCK-CCF	-3.20	100.08	111.68
2	b	901	BWC	CAL-CAJ-CAI	3.14	132.60	119.96
2	b	901	BWC	OAK-CAI-NAH	-3.13	121.39	126.36
3	b	902	25L	OAM-PCT-OBK	2.92	114.49	106.73
2	a	801	BWC	OAK-CAI-NAH	-2.87	121.81	126.36
3	a	802	25L	N6-C6-N1	-2.78	112.81	118.57
3	a	802	25L	OBT-PCT-OAM	2.67	117.86	107.64
2	b	901	BWC	CAD-CAE-CAJ	2.65	108.38	106.64
2	a	801	BWC	CAE-CAJ-CAL	-2.54	120.38	132.05
3	b	902	25L	OBT-PCT-OBK	-2.50	100.07	106.73
2	a	801	BWC	OAU-CAT-CAP	-2.49	117.19	120.95
3	a	802	25L	CCG-CCL-CCO	2.49	107.56	102.89
2	b	901	BWC	CBA-CBB-CBC	-2.38	98.45	105.19
2	a	801	BWC	CAW-NAV-CAT	2.36	127.45	122.08
3	b	902	25L	PCU-OBK-CCL	2.33	127.87	119.41
2	a	801	BWC	CBA-CBB-CBC	-2.30	98.70	105.19
3	b	902	25L	C5'-C4'-C3'	-2.27	106.67	115.18
2	b	901	BWC	CAE-CAJ-CAL	-2.23	121.81	132.05
3	a	802	25L	C1'-N9-C4	-2.22	122.73	126.64
3	b	902	25L	OBK-CCL-CCG	-2.11	104.04	111.68
2	a	801	BWC	CAP-CAT-NAV	2.06	119.70	115.62
4	a	803	PO4	O4-P-O1	-2.04	103.42	110.89
3	b	902	25L	CCG-CCL-CCO	2.00	106.65	102.89

There are no chirality outliers.

All (19) torsion outliers are listed below:

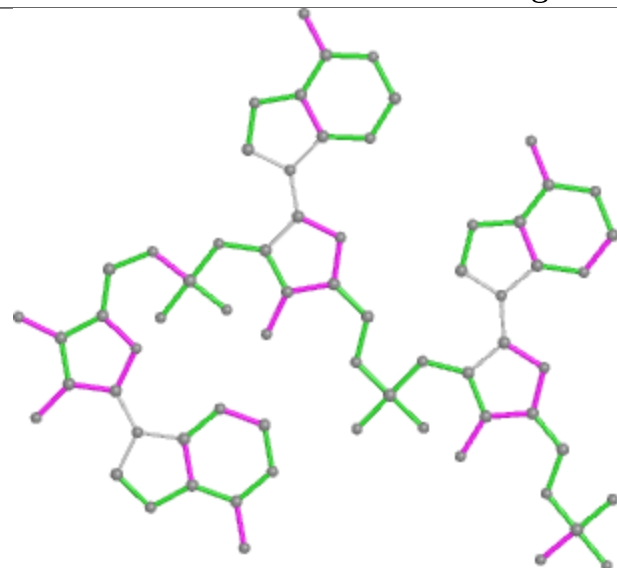
Mol	Chain	Res	Type	Atoms
2	a	801	BWC	CAW-CAX-NAY-CAZ
3	b	902	25L	O4'-C4'-C5'-O5'
3	b	902	25L	CBA-OBM-PCV-OAG
2	a	801	BWC	NAV-CAW-CAX-NAY
2	b	901	BWC	NAV-CAW-CAX-NAY
3	b	902	25L	OBM-CBA-CCJ-OBP
3	b	902	25L	OBM-CBA-CCJ-CCG
3	b	902	25L	C3'-C4'-C5'-O5'
3	b	902	25L	C5'-O5'-PCU-OBP
3	b	902	25L	CBA-OBM-PCV-OBQ
3	b	902	25L	CCL-OBP-PCU-O5'
2	a	801	BWC	CAX-CAW-NAV-CAT
3	b	902	25L	CCO-CCL-OBP-PCU
3	b	902	25L	C5'-O5'-PCU-OAF
3	b	902	25L	C5'-O5'-PCU-OAP
3	a	802	25L	C3'-C4'-C5'-O5'
3	b	902	25L	CCG-CCL-OBP-PCU
3	a	802	25L	O4'-C4'-C5'-O5'
3	a	802	25L	CBA-OBM-PCV-OAQ

There are no ring outliers.

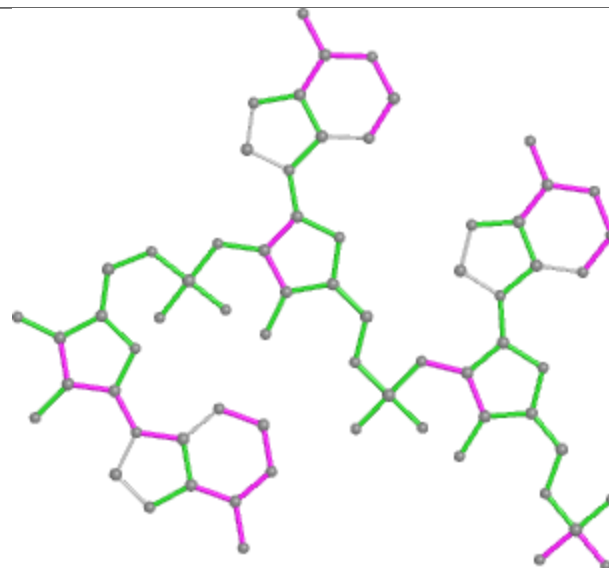
No monomer is involved in short contacts.

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.

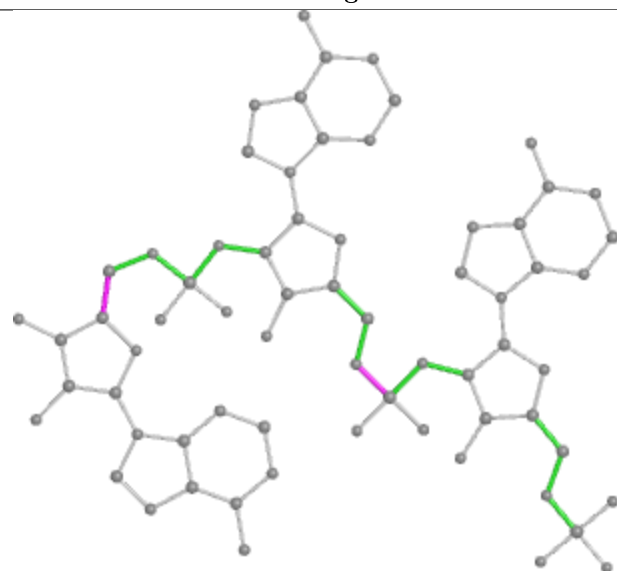
Ligand 25L a 802



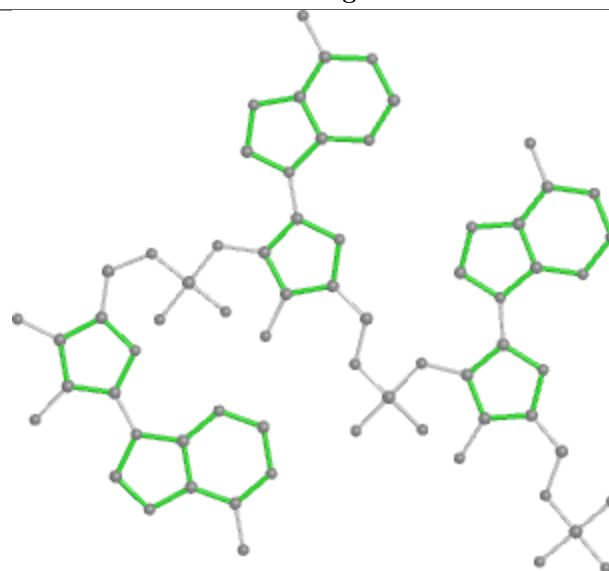
Bond lengths



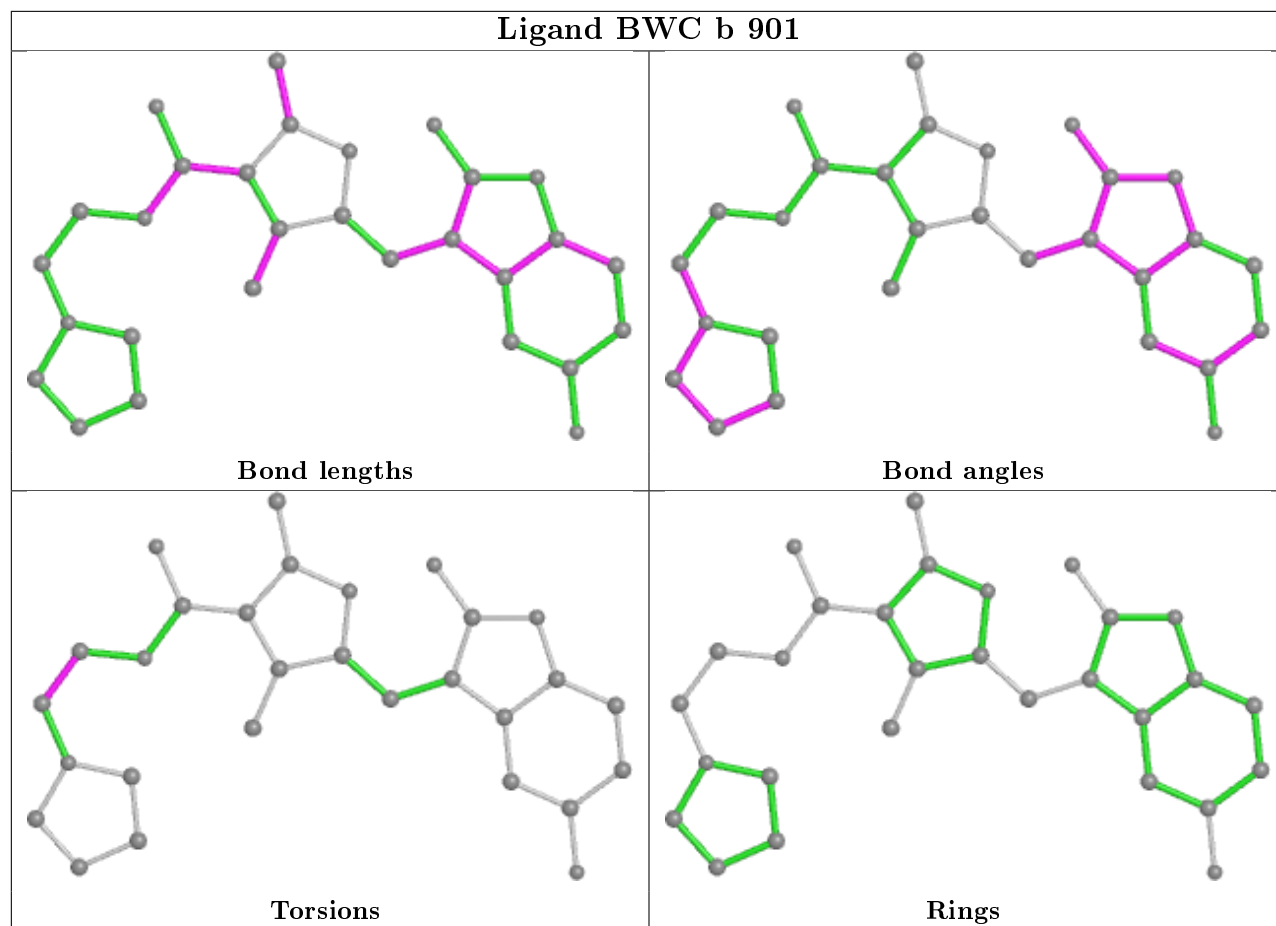
Bond angles

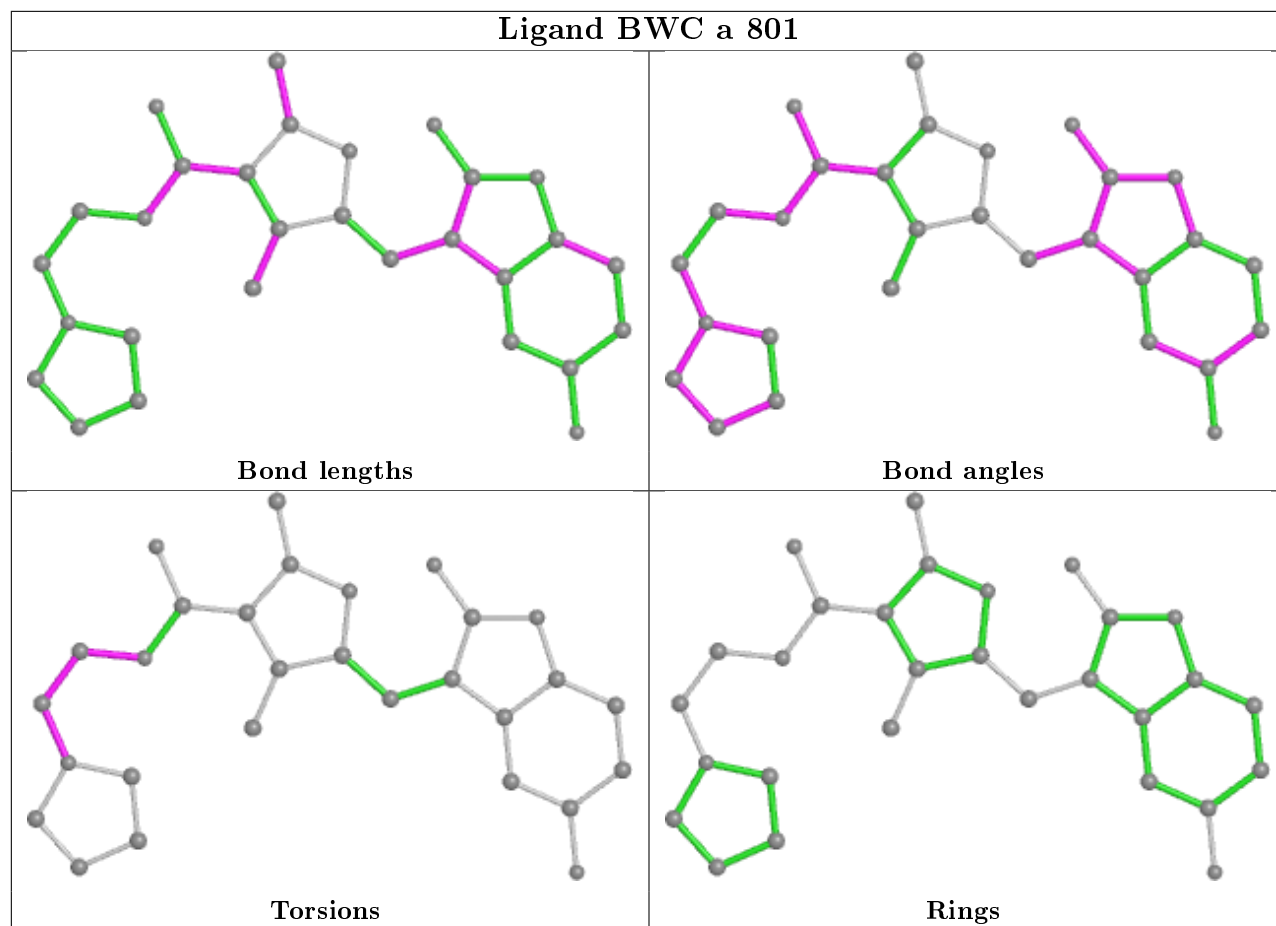


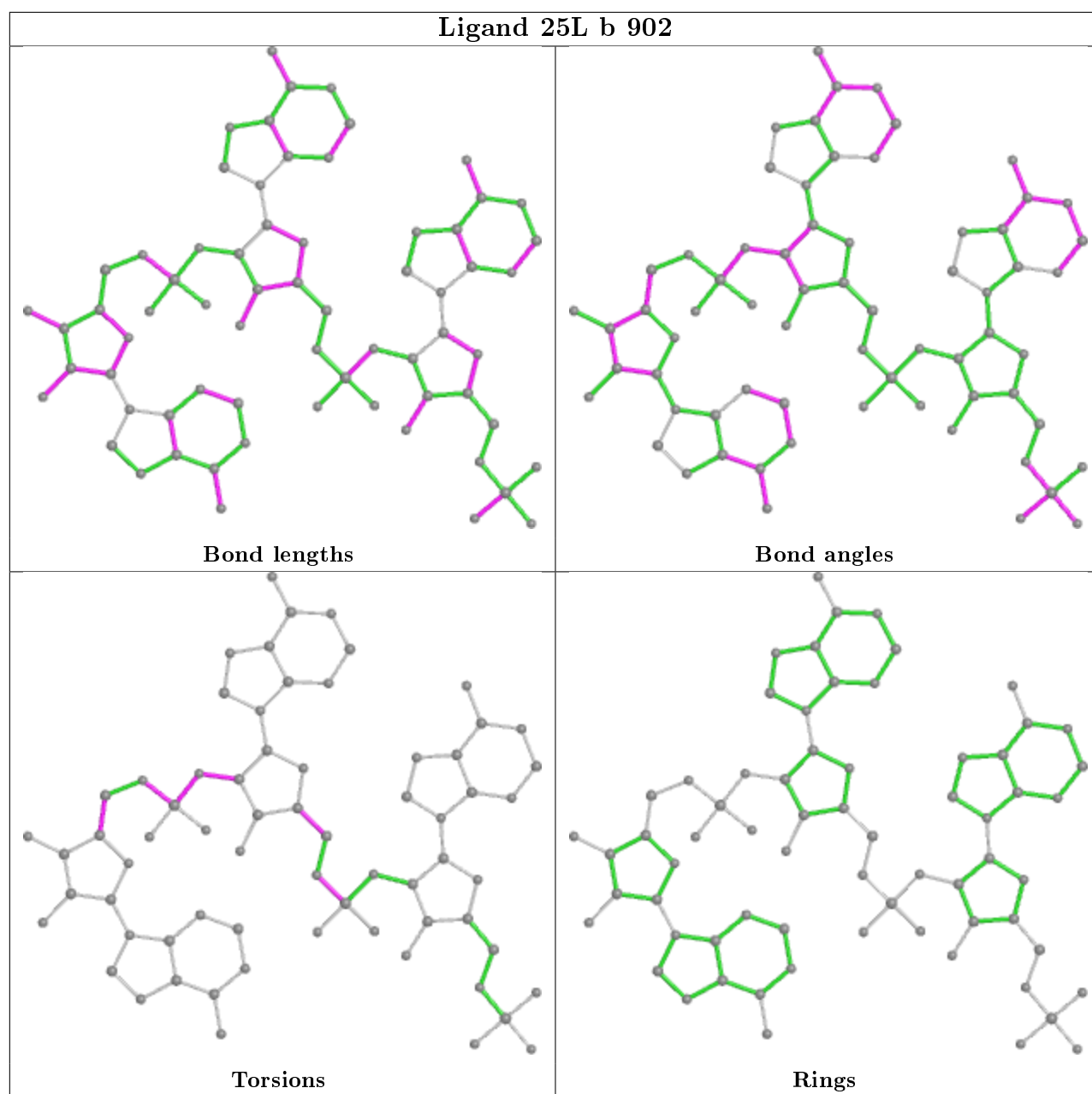
Torsions



Rings







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, 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	a	681/717 (94%)	0.29	23 (3%) 45 54	50, 94, 131, 172	0
1	b	688/717 (95%)	0.48	51 (7%) 14 19	53, 98, 151, 198	0
All	All	1369/1434 (95%)	0.39	74 (5%) 25 32	50, 96, 142, 198	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	b	46	GLY	10.8
1	a	43	LEU	6.7
1	b	42	LEU	6.0
1	b	39	VAL	5.3
1	b	76	LEU	5.2
1	b	111	PRO	5.2
1	b	47	ALA	4.9
1	b	107	GLN	4.8
1	b	49	ALA	4.8
1	a	299	CYS	4.6
1	b	73	VAL	4.6
1	a	310	TYR	4.6
1	b	140	ARG	4.5
1	b	83	PRO	4.1
1	b	64	ALA	4.0
1	a	40	ARG	3.9
1	b	190	LYS	3.9
1	b	106	LEU	3.7
1	b	620	SER	3.6
1	b	61	LEU	3.5
1	b	256	LEU	3.5
1	b	97	ALA	3.4
1	b	96	ILE	3.3
1	b	567	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	b	144	GLU	3.2
1	a	41	GLN	3.1
1	b	35	ASP	3.0
1	b	661	ASN	3.0
1	b	142	LEU	3.0
1	b	619	THR	3.0
1	b	662	LEU	3.0
1	a	76	LEU	2.9
1	a	623	SER	2.9
1	b	78	LYS	2.9
1	a	142	LEU	2.8
1	b	621	GLU	2.8
1	a	283	LEU	2.8
1	b	40	ARG	2.8
1	b	208	LEU	2.6
1	a	719	GLU	2.6
1	b	94	PHE	2.6
1	b	31	VAL	2.6
1	b	185	LEU	2.5
1	a	39	VAL	2.5
1	b	570	VAL	2.5
1	a	80	GLY	2.5
1	a	44	GLU	2.5
1	b	264	VAL	2.4
1	b	277	LEU	2.4
1	a	34	ALA	2.4
1	a	49	ALA	2.4
1	b	544	PHE	2.4
1	b	30	ALA	2.4
1	a	303	VAL	2.3
1	b	109	LEU	2.3
1	b	34	ALA	2.3
1	b	252	LEU	2.2
1	b	639	GLU	2.2
1	b	205	VAL	2.2
1	a	571	GLU	2.2
1	a	48	ASP	2.2
1	b	58	TRP	2.2
1	a	84	CYS	2.2
1	b	99	ILE	2.1
1	b	27	LEU	2.1
1	b	44	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	a	187	HIS	2.1
1	b	285	GLU	2.1
1	b	60	PRO	2.0
1	b	326	ASP	2.0
1	a	293	ARG	2.0
1	a	319	ARG	2.0
1	b	186	LEU	2.0
1	a	51	PHE	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 [i](#)

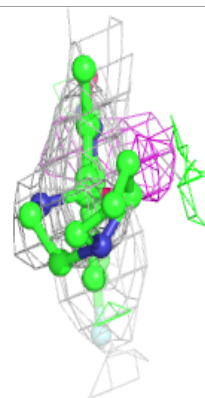
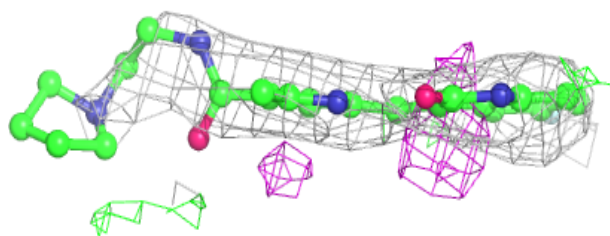
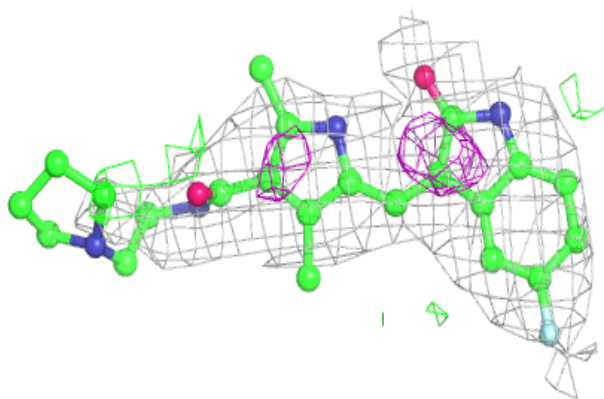
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BWC	a	801	29/29	0.85	0.30	85,102,180,181	0
2	BWC	b	901	29/29	0.87	0.39	95,134,172,174	0
3	25L	b	902	67/75	0.93	0.16	71,95,139,141	0
3	25L	a	802	67/75	0.96	0.15	62,77,91,101	0
4	PO4	a	803	5/5	0.97	0.12	68,74,84,85	0

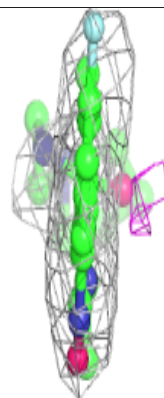
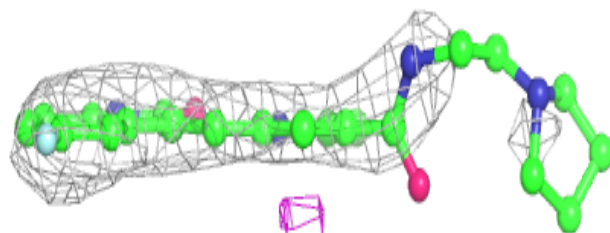
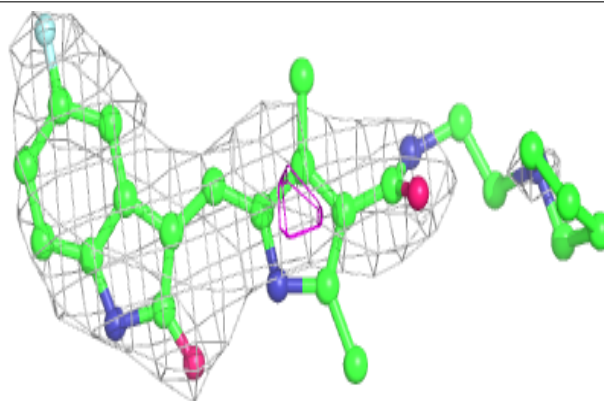
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BWC a 801:

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

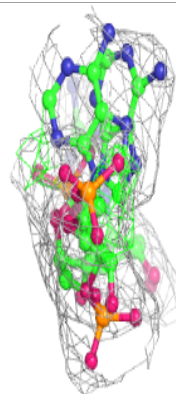
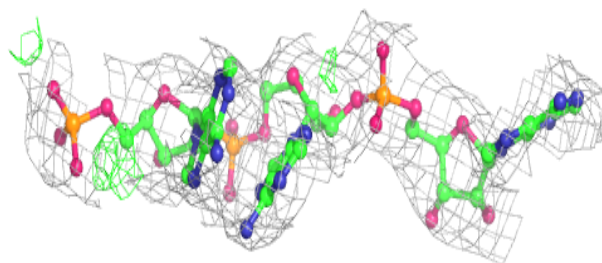
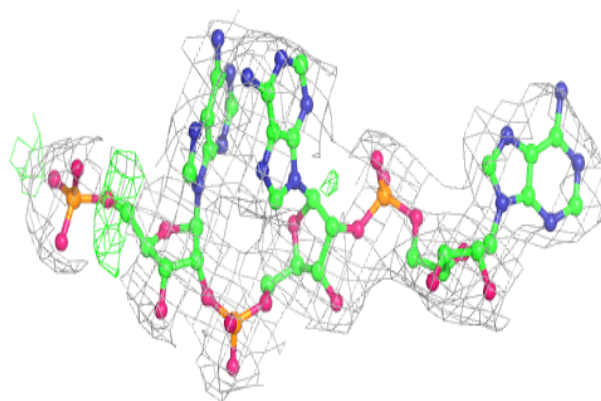
**Electron density around BWC b 901:**

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

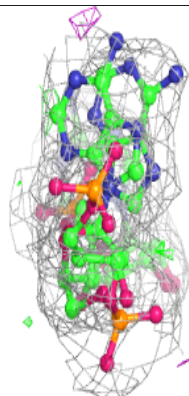
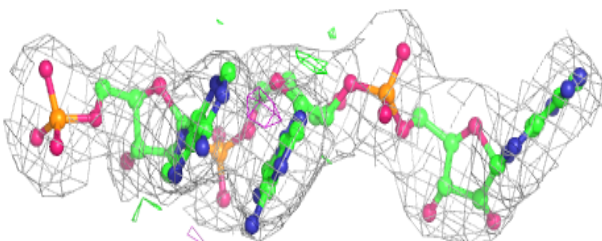
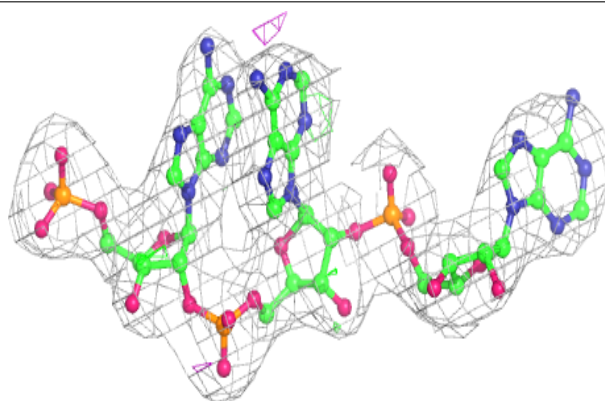


Electron density around 25L b 902:

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

**Electron density around 25L a 802:**

$2mF_o-DF_c$ (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.