



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 11:46 AM BST

PDB ID : 6M11
Title : Crystal structure of Rnase L in complex with Sunitinib
Authors : Tang, J.; Huang, H.
Deposited on : 2020-02-24
Resolution : 2.46 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

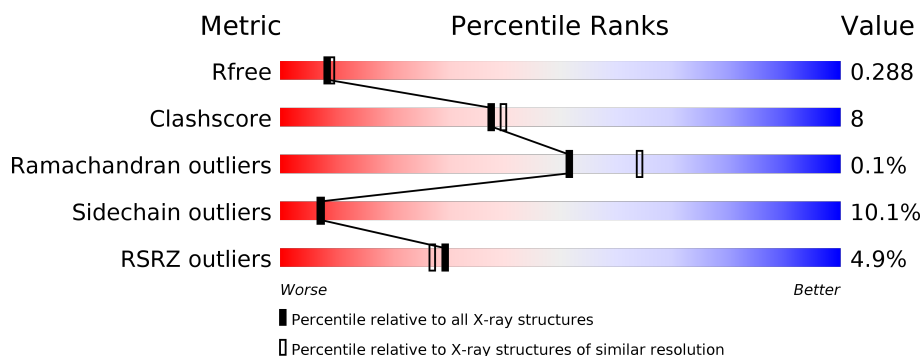
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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>4%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	b	717	<div> <div>5%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11176 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.

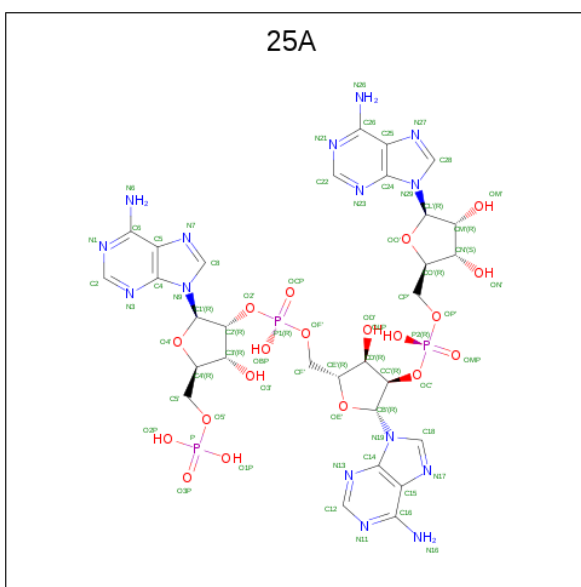
- Molecule 1 is a protein called Ribonuclease L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	681	Total	C	N	O	S	0	0	0
			5408	3396	955	1035	22			
1	b	684	Total	C	N	O	S	0	0	0
			5418	3400	955	1041	22			

There are 10 discrepancies between the modelled and reference sequences:

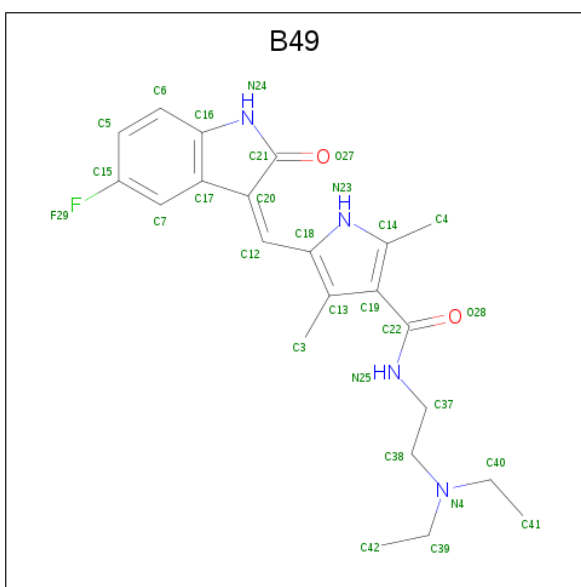
Chain	Residue	Modelled	Actual	Comment	Reference
a	16	GLY	-	expression tag	UNP A5H025
a	17	ALA	-	expression tag	UNP A5H025
a	18	MET	-	expression tag	UNP A5H025
a	19	ASP	-	expression tag	UNP A5H025
a	20	PRO	-	expression tag	UNP A5H025
b	16	GLY	-	expression tag	UNP A5H025
b	17	ALA	-	expression tag	UNP A5H025
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'-O-MONOPHOSPHORYLADENYLYL(2'->5')ADENYLYL(2'->5')ADENOSINE (three-letter code: 25A) (formula: C₃₀H₃₈N₁₅O₁₉P₃).



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

- Molecule 3 is N-[2-(diethylamino)ethyl]-5-[(Z)-(5-fluoro-2-oxo-1,2-dihydro-3H-indol-3-ylidene)methyl]-2,4-dimethyl-1H-pyrrole-3-carboxamide (three-letter code: B49) (formula: C₂₂H₂₇FN₄O₂) (labeled as "Ligand of Interest" by author).



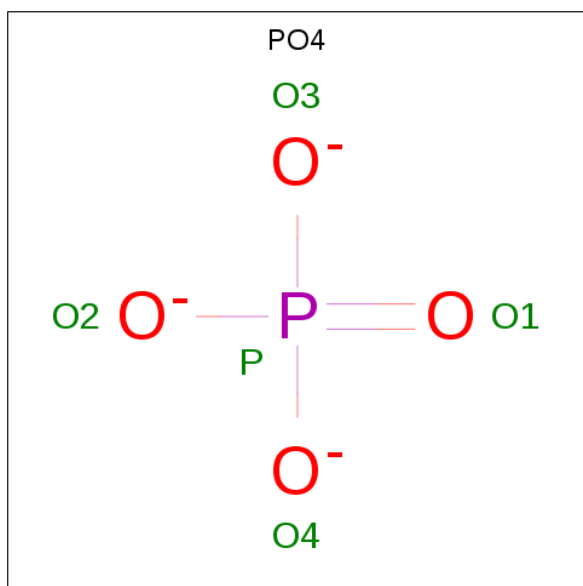
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	a	1	Total	C	F	N	O	0	0
			29	22	1	4	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	b	1	Total	C	F	N	O	0	0
			29	22	1	4	2		

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	a	81	Total	O	0	0
			81	81		
5	b	72	Total	O	0	0
			72	72		

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.

Chain a:

4% 87% 7% 5%

GLY
ALA
MET
ASP
PRO
ALA
S22
L23
M26
I36
E37
Q38
V39
R40
L43
E44
A47
F51
L61
D71
L76
C94
F94
T100
Y103
L106
Q107
L108
L109
E137
A138
L139
R140
F141
L142
L170
M171
D172
R221
L222
L223
E235
Y238

S237
D251
Q259
E260
V264
E270
T273
A274
L275
L276
L277
T297
L320
A323
G324
GLU
D326
F327
R328
P329
P331
E332
N333
E343
A344
L345
M355
D371
E374
D384
E402
L428
R447
E472
S476
K493
T496
D502

E509
D510
K513
L521
G567
ASP
ASN
VAL
E571
D572
R573
L574
D601
I602
M608
L614
L615
Q616
P617
GLY
THR
S620
Q628
K632
L633
M638
A643
TYR
TYR
LYS
LYS
ILE
SER
LYS
LYS
LYS
LYS
ALA
LYS
HIS
THR
ASN
GLU
GLY
ASN
L662
L667

Chain b:

GLY	ALA	MET	ASP	PRO	ALA	SER	L23	E24	E25	H26	L27	T28	Q29	D35	I36	E37	Q38	V39	L42	L43	E44	R45	G46	S63	A64	D71	L72	V73	A74	L75	L76	P83	I95	I96	A97	G98	I99	T100	G101	M102	V103	L106	Q107	L108	L109	L110	F111	E118	G119	D120
F127	A130	E135	V136	E137	A138	L139	R140	F141	L142	L143	E144	Q157	L170	L185	K190	M199	L223	H226	V230	E235	G236	S237	L256	E260	V264	V285	D286	E270	T273	A274	L275	L276	L277	R282	L320	H321	LYS	A323	R326	E327										
ARG	P329	P330	A331	GLU	R333	K334	K335	E343	A344	L345	I377	R391	LYS	F392	S393	S394	G395	LYS	LYS	LYS	ALA	LYS	HIS	THR	ASN	L428	T438	N453	S476	K493	T496	D500	D510	P511	Q512	K513	K540	D568	M569	V570	E571	L574	D601	L614	L615					

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.24Å 111.00Å 262.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.26 – 2.46 51.26 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.3 (51.26-2.46) 99.3 (51.26-2.46)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.220 , 0.285 0.221 , 0.288	Depositor DCC
R_{free} test set	3223 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11176	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 25A, B49

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	0.66	0/5501	0.88	7/7422 (0.1%)
1	b	0.65	0/5512	0.88	8/7438 (0.1%)
All	All	0.65	0/11013	0.88	15/14860 (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	a	0	1
1	b	0	1
All	All	0	2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	675	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	b	391	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	b	500	ASP	N-CA-C	6.02	127.24	111.00
1	b	120	ASP	CB-CG-OD1	5.99	123.69	118.30
1	a	510	ASP	CB-CG-OD1	5.94	123.64	118.30
1	b	320	LEU	CA-CB-CG	5.82	128.68	115.30
1	a	172	ASP	CB-CG-OD1	5.73	123.46	118.30
1	b	675	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	a	447	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	a	601	ASP	CB-CG-OD1	5.33	123.10	118.30
1	a	345	LEU	CB-CG-CD1	5.24	119.91	111.00
1	a	221	ARG	CA-CB-CG	5.19	124.82	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	170	LEU	CA-CB-CG	5.10	127.04	115.30
1	b	345	LEU	CB-CG-CD1	5.05	119.59	111.00
1	b	106	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	726	LYS	Peptide
1	b	615	LEU	Peptide

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	5408	0	5324	0	0
1	b	5418	0	5298	0	0
2	a	67	0	32	0	0
2	b	67	0	32	0	0
3	a	29	0	27	0	0
3	b	29	0	27	0	0
4	b	5	0	0	0	0
5	a	81	0	0	0	0
5	b	72	0	0	0	0
All	All	11176	0	10740	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 8.

There are no clashes within the asymmetric unit.

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	669/717 (93%)	630 (94%)	38 (6%)	1 (0%)	51	64
1	b	671/717 (94%)	626 (93%)	45 (7%)	0	100	100
All	All	1340/1434 (93%)	1256 (94%)	83 (6%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	327	PHE

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	581/617 (94%)	525 (90%)	56 (10%)	8	8
1	b	579/617 (94%)	518 (90%)	61 (10%)	7	6
All	All	1160/1234 (94%)	1043 (90%)	117 (10%)	7	7

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	23	LEU
1	a	26	MET
1	a	38	GLN
1	a	71	ASP
1	a	100	THR

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Mol	Chain	Res	Type
1	a	137	GLU
1	a	170	LEU
1	a	221	ARG
1	a	223	LEU
1	a	235	GLU
1	a	237	SER
1	a	251	ASP
1	a	259	GLN
1	a	260	GLU
1	a	264	VAL
1	a	270	GLU
1	a	273	THR
1	a	275	LEU
1	a	277	LEU
1	a	297	THR
1	a	320	LEU
1	a	327	PHE
1	a	328	ARG
1	a	333	ASN
1	a	343	GLU
1	a	345	LEU
1	a	371	ASP
1	a	384	ASP
1	a	428	LEU
1	a	472	GLU
1	a	476	SER
1	a	493	LYS
1	a	496	THR
1	a	502	ASP
1	a	513	LYS
1	a	521	LEU
1	a	572	ASP
1	a	573	ARG
1	a	574	LEU
1	a	601	ASP
1	a	608	ASN
1	a	614	LEU
1	a	616	GLN
1	a	628	GLN
1	a	632	LYS
1	a	633	ILE
1	a	638	MET

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Mol	Chain	Res	Type
1	a	670	LEU
1	a	671	LEU
1	a	675	ARG
1	a	685	LYS
1	a	688	LYS
1	a	702	GLU
1	a	703	LYS
1	a	726	LYS
1	a	727	THR
1	b	28	THR
1	b	29	GLN
1	b	43	LEU
1	b	44	GLU
1	b	63	SER
1	b	71	ASP
1	b	100	THR
1	b	103	VAL
1	b	110	LEU
1	b	118	GLU
1	b	135	ARG
1	b	137	GLU
1	b	157	GLN
1	b	170	LEU
1	b	199	MET
1	b	223	LEU
1	b	226	HIS
1	b	235	GLU
1	b	237	SER
1	b	260	GLU
1	b	264	VAL
1	b	270	GLU
1	b	273	THR
1	b	275	LEU
1	b	277	LEU
1	b	282	ARG
1	b	335	LYS
1	b	343	GLU
1	b	345	LEU
1	b	377	ILE
1	b	393	SER
1	b	394	GLU
1	b	396	SER

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Mol	Chain	Res	Type
1	b	401	GLN
1	b	404	SER
1	b	408	SER
1	b	428	LEU
1	b	438	THR
1	b	453	ASN
1	b	476	SER
1	b	493	LYS
1	b	496	THR
1	b	512	GLN
1	b	513	LYS
1	b	540	LYS
1	b	569	ASN
1	b	571	GLU
1	b	574	LEU
1	b	601	ASP
1	b	614	LEU
1	b	635	SER
1	b	639	GLU
1	b	642	ASN
1	b	670	LEU
1	b	671	LEU
1	b	672	LYS
1	b	675	ARG
1	b	685	LYS
1	b	688	LYS
1	b	703	LYS
1	b	726	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	29	GLN
1	a	159	GLN
1	a	198	ASN
1	a	210	ASN
1	a	429	HIS
1	a	481	GLN
1	a	616	GLN
1	b	29	GLN
1	b	226	HIS
1	b	442	HIS

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Mol	Chain	Res	Type
1	b	453	ASN
1	b	481	GLN
1	b	569	ASN
1	b	607	GLN
1	b	616	GLN
1	b	686	ASN

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	$\# Z > 2$
4	PO4	b	803	-	4,4,4	1.06	0	6,6,6	0.76	0
3	B49	b	802	-	27,31,31	2.78	5 (18%)	32,44,44	2.92	14 (43%)
2	25A	b	801	-	64,75,75	2.87	11 (17%)	75,116,116	2.20	16 (21%)
2	25A	a	1000	-	64,75,75	2.59	9 (14%)	75,116,116	2.34	16 (21%)
3	B49	a	1001	-	27,31,31	2.90	6 (22%)	32,44,44	2.92	15 (46%)

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	B49	b	802	-	-	4/14/30/30	0/3/3/3
2	25A	b	801	-	-	11/28/88/88	0/9/9/9
2	25A	a	1000	-	-	3/28/88/88	0/9/9/9
3	B49	a	1001	-	-	7/14/30/30	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	801	25A	C22-N23	10.34	1.48	1.32
3	a	1001	B49	C12-C20	9.33	1.48	1.34
2	b	801	25A	C2-N3	9.31	1.47	1.32
2	b	801	25A	C12-N13	9.31	1.47	1.32
2	a	1000	25A	C22-N23	9.29	1.47	1.32
3	b	802	B49	C12-C20	9.28	1.48	1.34
3	a	1001	B49	C17-C16	8.77	1.52	1.41
2	a	1000	25A	C2-N3	8.45	1.45	1.32
3	b	802	B49	C17-C16	7.99	1.51	1.41
2	b	801	25A	C22-N21	7.74	1.48	1.33
2	a	1000	25A	C12-N13	7.71	1.44	1.32
2	a	1000	25A	C2-N1	7.50	1.47	1.33
2	b	801	25A	C12-N11	7.48	1.47	1.33
2	b	801	25A	C2-N1	7.31	1.47	1.33
2	a	1000	25A	C12-N11	7.24	1.47	1.33
2	a	1000	25A	C22-N21	7.23	1.47	1.33
3	a	1001	B49	C19-C13	5.29	1.48	1.39
3	b	802	B49	C19-C13	5.23	1.48	1.39
3	a	1001	B49	O27-C21	3.74	1.30	1.23
2	b	801	25A	OO'-CL'	3.53	1.46	1.41
2	b	801	25A	O4'-C1'	2.87	1.45	1.41
3	b	802	B49	O27-C21	2.87	1.29	1.23
2	b	801	25A	C5-C4	2.72	1.48	1.40
2	b	801	25A	C25-C24	2.56	1.47	1.40
3	a	1001	B49	C7-C15	2.55	1.42	1.37
2	b	801	25A	C15-C14	2.53	1.47	1.40
2	a	1000	25A	C15-C14	2.41	1.47	1.40
3	b	802	B49	C5-C15	2.33	1.41	1.37
2	a	1000	25A	C25-C24	2.25	1.46	1.40
2	a	1000	25A	O4'-C1'	2.19	1.44	1.41
3	a	1001	B49	C18-C12	2.07	1.49	1.41

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	802	B49	C20-C21-N24	10.44	112.73	106.88
3	a	1001	B49	C20-C21-N24	10.13	112.56	106.88
2	a	1000	25A	N23-C22-N21	-9.48	113.86	128.68
2	a	1000	25A	N3-C2-N1	-9.33	114.10	128.68
2	b	801	25A	N3-C2-N1	-9.02	114.58	128.68
2	b	801	25A	N23-C22-N21	-8.64	115.18	128.68
2	a	1000	25A	N13-C12-N11	-8.24	115.80	128.68
2	b	801	25A	N13-C12-N11	-8.13	115.98	128.68
3	a	1001	B49	C16-N24-C21	-5.27	108.07	111.38
3	a	1001	B49	C6-C16-C17	-4.96	117.21	122.19
3	b	802	B49	C7-C17-C16	4.62	123.85	119.42
3	b	802	B49	C6-C5-C15	4.29	122.80	118.36
2	b	801	25A	OD'-CD'-CC'	4.22	123.14	111.17
2	a	1000	25A	C2-N1-C6	4.08	125.73	118.75
3	a	1001	B49	C6-C5-C15	4.07	122.57	118.36
3	b	802	B49	C12-C20-C21	4.05	136.24	119.96
3	b	802	B49	C6-C16-C17	-4.05	118.13	122.19
3	b	802	B49	C16-N24-C21	-3.91	108.92	111.38
3	a	1001	B49	C12-C20-C21	3.87	135.53	119.96
2	a	1000	25A	O1P-P-O3P	3.55	124.58	110.68
3	a	1001	B49	C16-C17-C20	-3.47	104.36	106.64
3	a	1001	B49	O28-C22-C19	-3.38	115.86	120.95
2	a	1000	25A	OBP-P1-OC	3.24	128.28	112.24
2	b	801	25A	C2-N1-C6	3.23	124.28	118.75
3	b	802	B49	C3-C13-C19	3.17	130.62	124.68
2	a	1000	25A	C12-N11-C16	3.10	124.06	118.75
2	b	801	25A	C14-C15-N17	-3.10	106.16	109.40
3	b	802	B49	C17-C20-C21	-3.09	103.53	105.30
2	a	1000	25A	P1-O2'-C2'	3.03	130.44	119.41
3	a	1001	B49	C7-C17-C16	3.00	122.29	119.42
3	a	1001	B49	C19-C22-N25	2.98	121.54	115.62
2	a	1000	25A	C22-N21-C26	2.95	123.80	118.75
2	b	801	25A	O1P-P-O3P	2.93	122.14	110.68
2	a	1000	25A	OLP-P2-OMP	2.86	126.39	112.24
2	a	1000	25A	OC'-P2-OMP	-2.82	98.87	109.47
2	b	801	25A	OC'-CC'-CD'	2.79	121.79	111.68
2	a	1000	25A	C24-C25-N27	-2.77	106.51	109.40
2	a	1000	25A	C1'-N9-C4	-2.68	121.94	126.64
2	a	1000	25A	OD'-CD'-CE'	-2.65	103.39	111.05
3	b	802	B49	C17-C20-C12	-2.59	120.15	132.05
2	b	801	25A	C12-N11-C16	2.54	123.10	118.75
2	b	801	25A	C2'-C3'-C4'	2.53	107.49	101.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1001	B49	C17-C20-C12	-2.52	120.47	132.05
3	a	1001	B49	C3-C13-C19	2.50	129.36	124.68
3	b	802	B49	O27-C21-C20	-2.49	124.44	127.71
3	a	1001	B49	C17-C20-C21	-2.49	103.87	105.30
3	a	1001	B49	C17-C16-N24	2.48	111.06	108.22
3	b	802	B49	O28-C22-C19	-2.48	117.22	120.95
2	b	801	25A	C22-N21-C26	2.47	122.98	118.75
3	a	1001	B49	O27-C21-N24	-2.41	122.53	126.36
2	b	801	25A	CC'-CD'-CE'	2.41	107.23	101.99
3	b	802	B49	C16-C17-C20	-2.38	105.07	106.64
2	b	801	25A	C25-C26-N26	-2.26	116.92	120.35
3	b	802	B49	C37-C38-N4	2.25	118.48	112.88
2	b	801	25A	CF'-CE'-CD'	-2.24	106.78	115.18
2	a	1000	25A	O2'-C2'-C1'	-2.24	102.04	110.10
2	b	801	25A	N26-C26-N21	2.24	123.21	118.57
3	b	802	B49	O27-C21-N24	-2.23	122.82	126.36
2	b	801	25A	CN'-CM'-CL'	2.23	104.33	100.98
3	a	1001	B49	O27-C21-C20	-2.15	124.89	127.71
2	a	1000	25A	O3'-C3'-C4'	-2.12	104.91	111.05

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	b	801	25A	C3'-C4'-C5'-O5'
2	b	801	25A	OE'-CE'-CF'-OF'
2	b	801	25A	CD'-CE'-CF'-OF'
2	b	801	25A	CP'-OP'-P2-OLP
2	a	1000	25A	CF'-OF'-P1-OBP
3	a	1001	B49	C19-C22-N25-C37
3	a	1001	B49	N25-C37-C38-N4
3	a	1001	B49	O28-C22-N25-C37
3	b	802	B49	N25-C37-C38-N4
2	b	801	25A	CN'-CO'-CP'-OP'
3	b	802	B49	C41-C40-N4-C38
3	a	1001	B49	C41-C40-N4-C39
3	b	802	B49	C41-C40-N4-C39
3	a	1001	B49	C41-C40-N4-C38
2	b	801	25A	O4'-C4'-C5'-O5'
3	a	1001	B49	C42-C39-N4-C40
3	a	1001	B49	C42-C39-N4-C38
2	b	801	25A	CP'-OP'-P2-OC'

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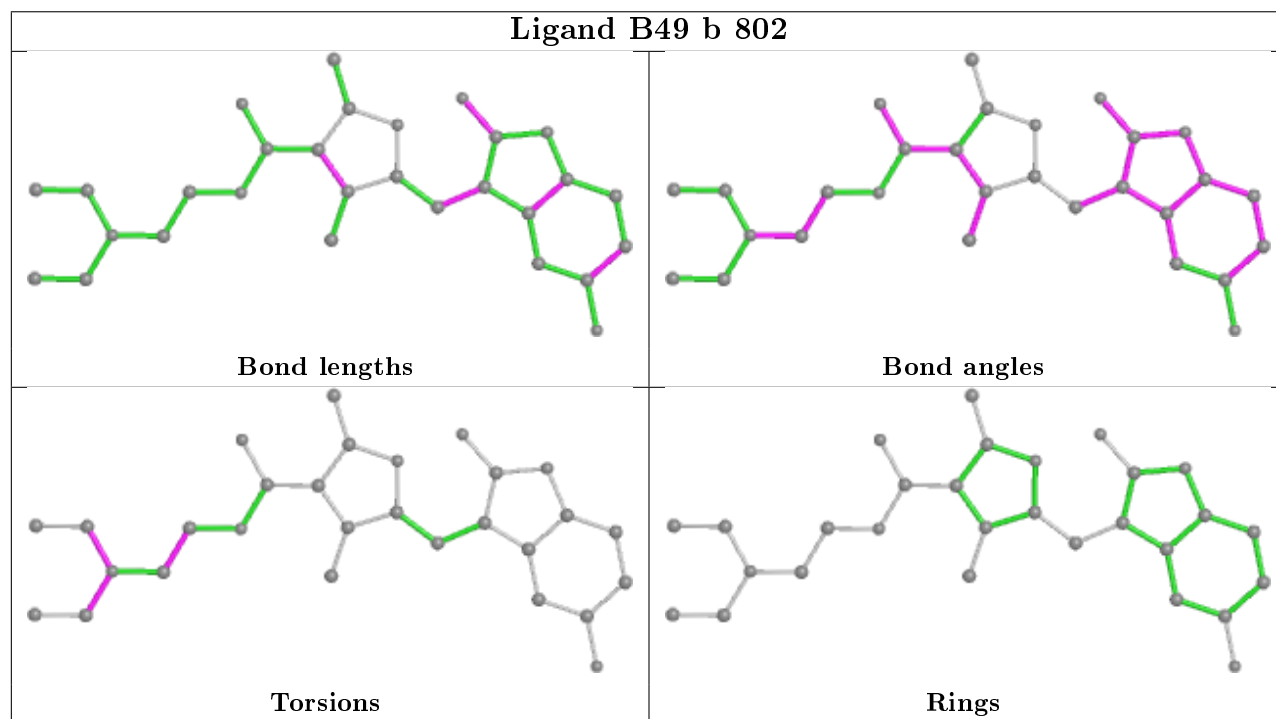
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Mol	Chain	Res	Type	Atoms
3	b	802	B49	C42-C39-N4-C40
2	b	801	25A	OO'-CO'-CP'-OP'
2	b	801	25A	CP'-OP'-P2-OMP
2	b	801	25A	CF'-OF'-P1-O2'
2	a	1000	25A	O4'-C4'-C5'-O5'
2	a	1000	25A	CF'-OF'-P1-OCP
2	b	801	25A	CD'-CC'-OC'-P2

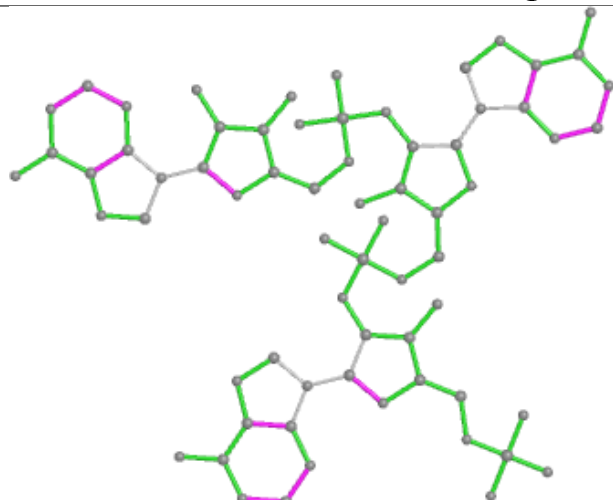
There are no ring outliers.

No monomer is involved in short contacts.

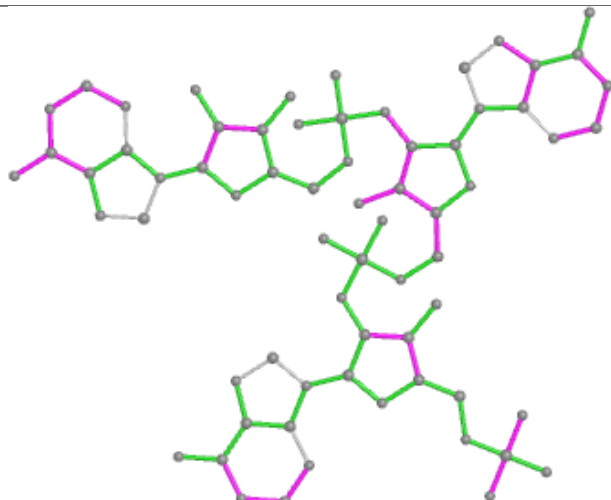
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



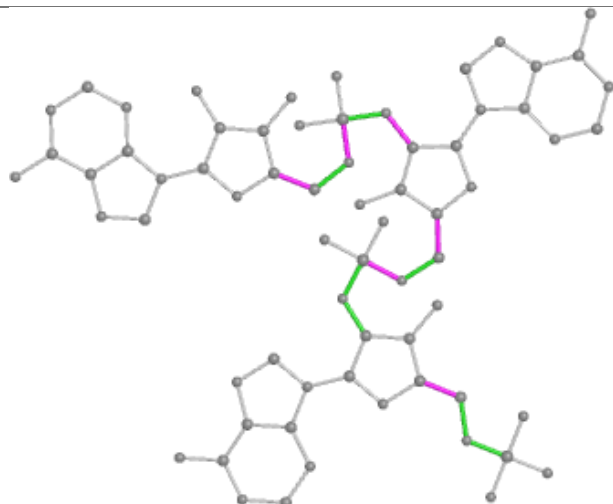
Ligand 25A b 801



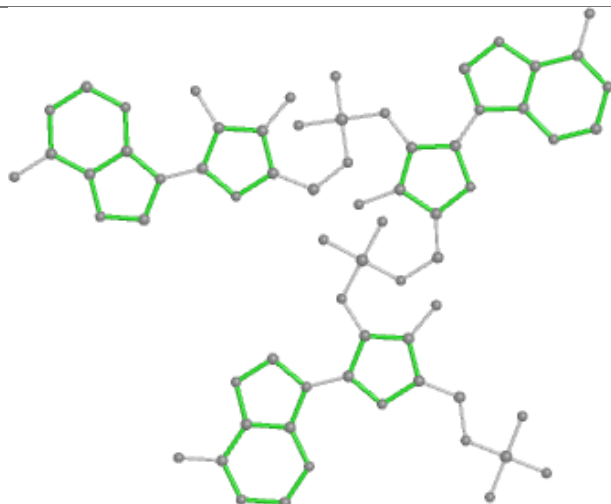
Bond lengths



Bond angles

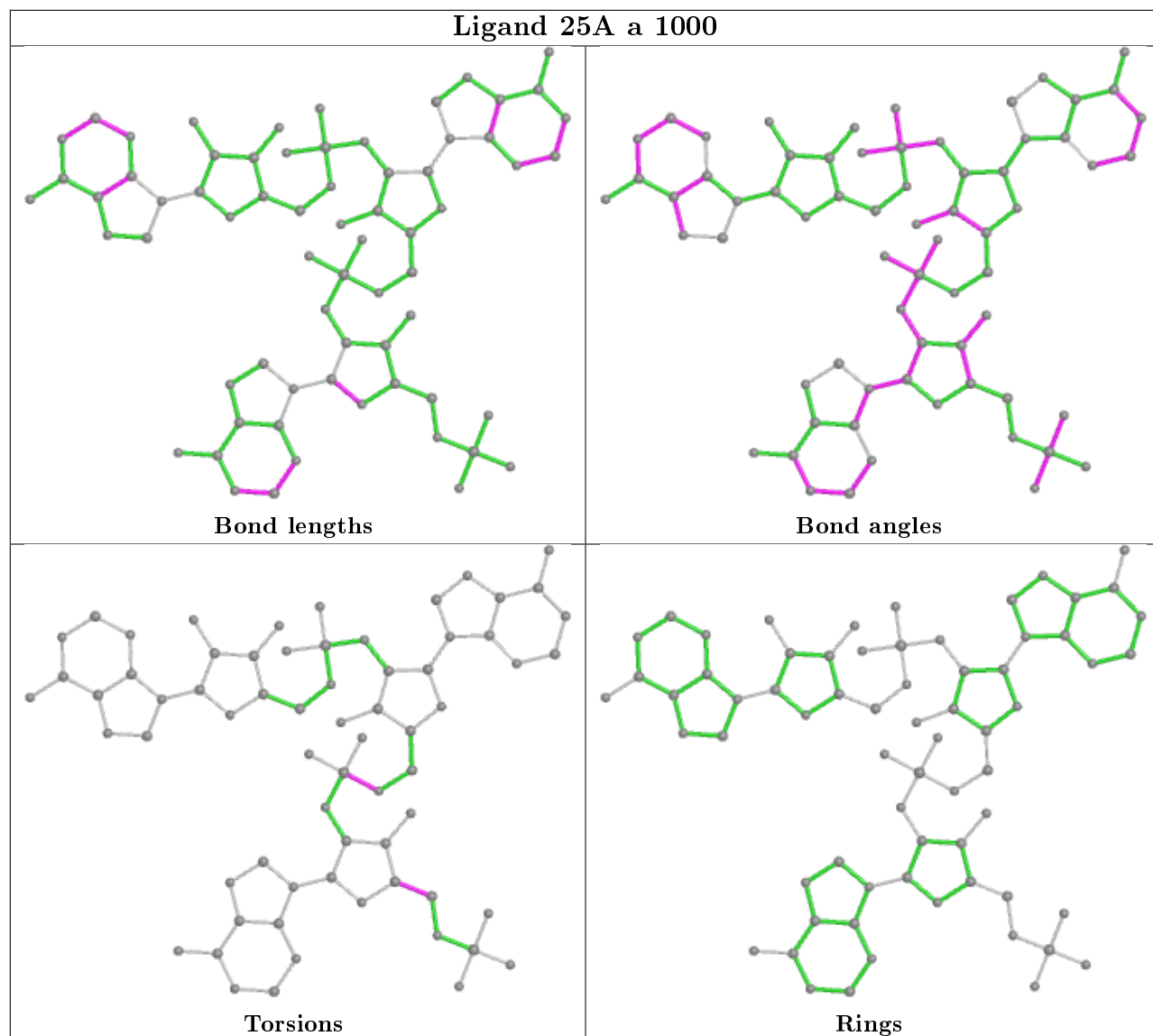


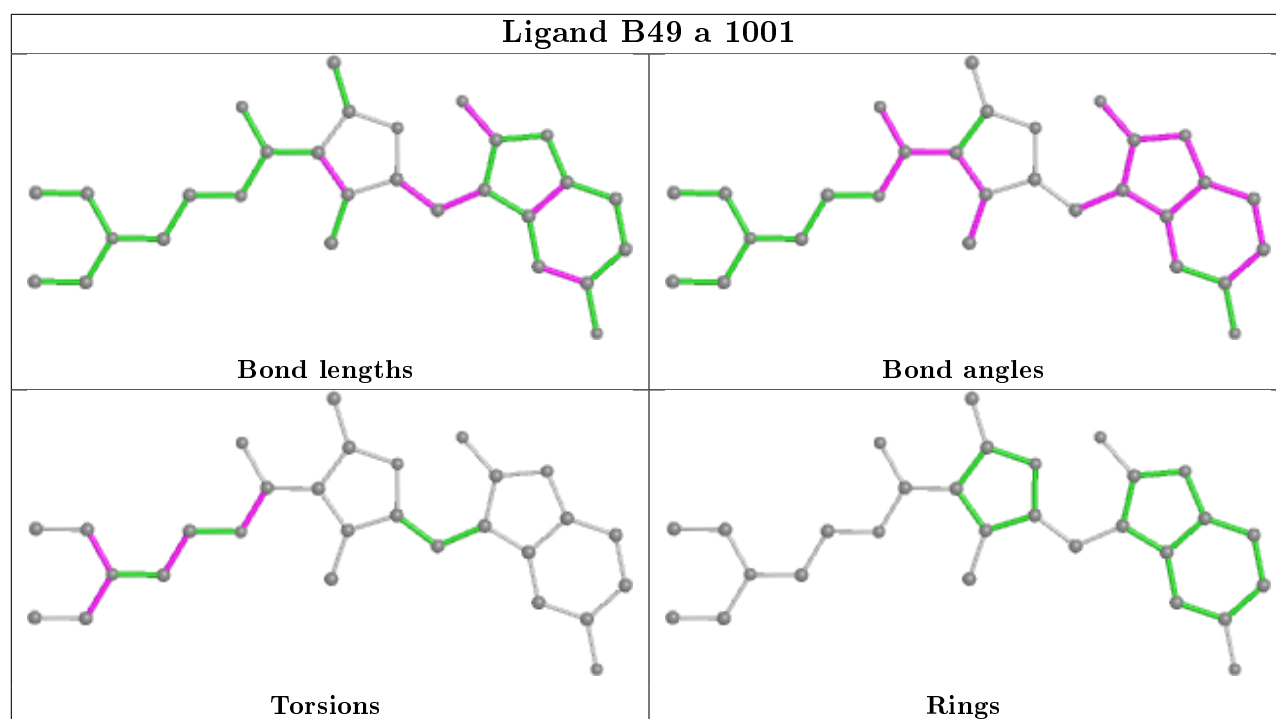
Torsions



Rings

Ligand 25A a 1000





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	28 (4%) 37 34	45, 85, 122, 161	0
1	b	684/717 (95%)	0.31	39 (5%) 23 20	46, 87, 138, 242	0
All	All	1365/1434 (95%)	0.30	67 (4%) 29 27	45, 86, 131, 242	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	43	LEU	7.2
1	a	139	LEU	5.9
1	b	39	VAL	5.4
1	a	323	ALA	4.6
1	b	99	ILE	4.3
1	a	106	LEU	4.3
1	a	509	GLU	4.2
1	b	106	LEU	4.2
1	b	139	LEU	4.1
1	a	324	GLY	4.1
1	b	36	ILE	3.9
1	b	76	LEU	3.8
1	b	109	LEU	3.7
1	b	26	MET	3.7
1	b	35	ASP	3.6
1	b	25	GLU	3.6
1	b	24	GLU	3.5
1	b	74	ALA	3.4
1	b	72	LEU	3.4
1	b	142	LEU	3.4
1	b	256	LEU	3.4
1	a	326	ASP	3.4
1	b	37	GLU	3.3
1	a	76	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	b	326	ASP	3.2
1	a	667	LEU	3.2
1	a	374	GLU	3.1
1	b	111	PRO	3.1
1	b	73	VAL	3.0
1	b	97	ALA	2.9
1	b	71	ASP	2.9
1	a	142	LEU	2.9
1	a	103	VAL	2.8
1	b	95	ILE	2.8
1	a	602	ILE	2.8
1	a	44	GLU	2.7
1	a	36	ILE	2.7
1	a	84	CYS	2.7
1	b	83	PRO	2.7
1	a	47	ALA	2.6
1	b	42	LEU	2.6
1	a	328	ARG	2.6
1	b	190	LYS	2.6
1	b	101	GLY	2.6
1	b	619	THR	2.5
1	a	94	PHE	2.4
1	a	109	LEU	2.4
1	a	141	PHE	2.4
1	a	51	PHE	2.4
1	b	266	ASP	2.4
1	b	185	LEU	2.4
1	a	61	LEU	2.4
1	b	127	PHE	2.3
1	b	510	ASP	2.3
1	b	144	GLU	2.3
1	a	107	GLN	2.2
1	b	568	ASP	2.2
1	b	130	ALA	2.2
1	a	40	ARG	2.1
1	b	140	ARG	2.1
1	b	46	GLY	2.1
1	a	355	MET	2.0
1	b	230	VAL	2.0
1	a	39	VAL	2.0
1	a	402	GLU	2.0
1	b	64	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	b	107	GLN	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](#)

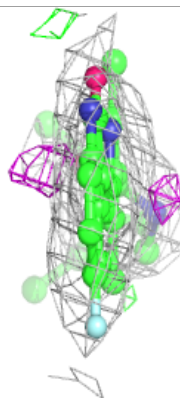
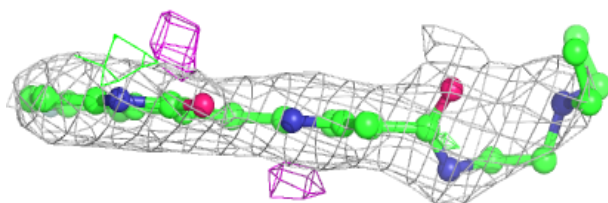
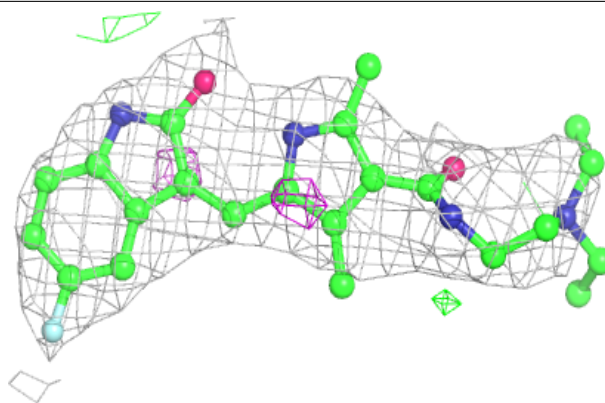
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	B49	a	1001	29/29	0.91	0.20	63,77,141,146	0
3	B49	b	802	29/29	0.92	0.19	74,96,116,124	0
2	25A	b	801	67/67	0.93	0.20	68,94,119,126	0
2	25A	a	1000	67/67	0.96	0.14	55,71,78,85	0
4	PO4	b	803	5/5	0.98	0.15	73,74,79,83	0

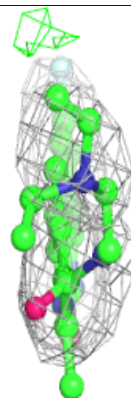
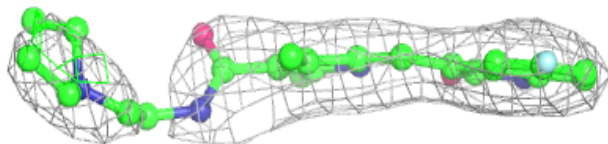
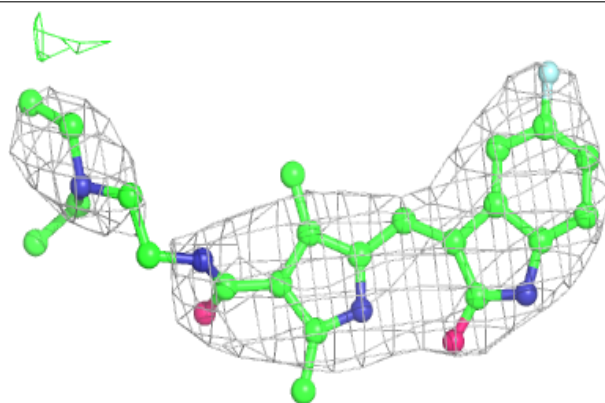
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B49 a 1001:

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

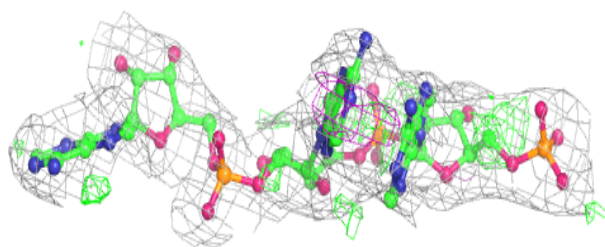
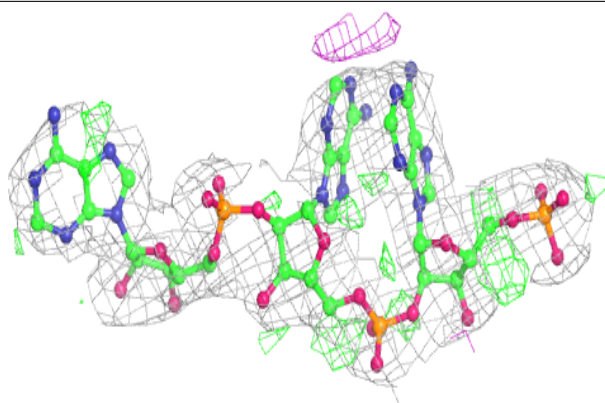
**Electron density around B49 b 802:**

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

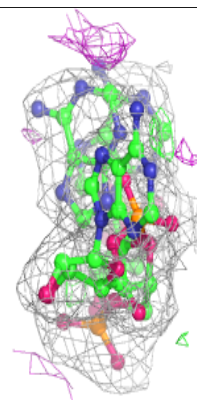
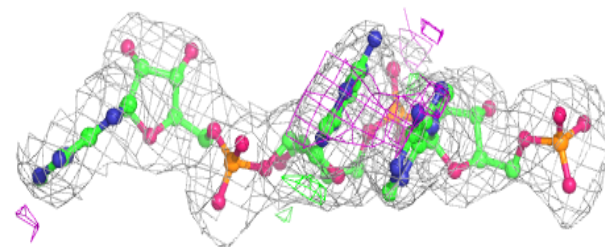
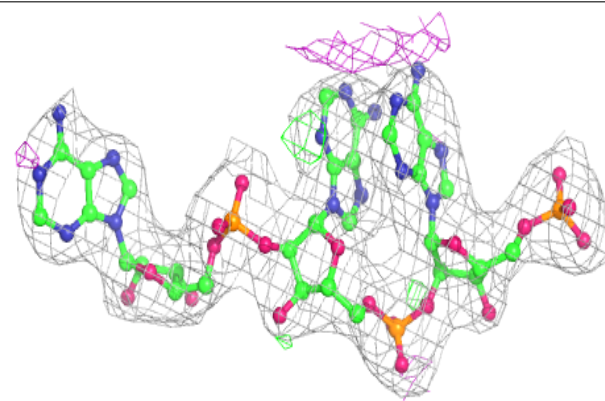


Electron density around 25A b 801:

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

**Electron density around 25A a 1000:**

$2mF_o-DF_c$ (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.