wwPDB X-ray Structure Validation Summary Report (i)

Apr 1, 2025 – 11:15 pm BST

PDB ID	:	5NPK / pdb_00005npk
Title	:	1.98A STRUCTURE OF THIOPHENE1 WITH S.AUREUS DNA GYRASE AND DNA
Authors	:	Bax, B.D.; Chan, P.F.; Stavenger, R.A.
Deposited on	:	2017-04-17
Resolution	:	1.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
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:

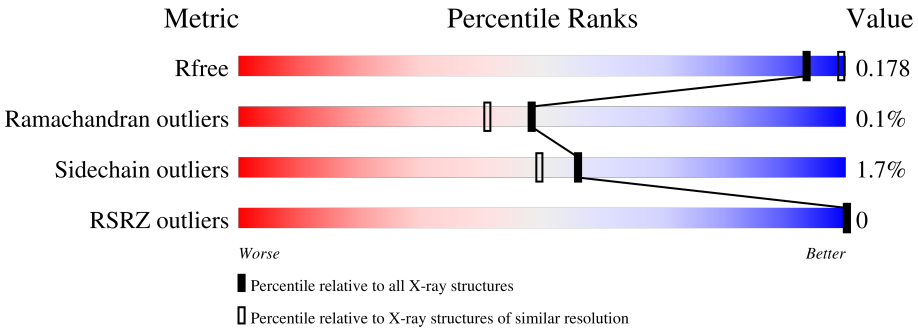
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 1.98 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}	164625	1356 (1.98-1.98)
Ramachandran outliers	177936	1426 (1.98-1.98)
Sidechain outliers	177891	1426 (1.98-1.98)
RSRZ outliers	164620	1356 (1.98-1.98)

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	B	692	91% 6% ·
1	D	692	92% · · ·
1	b	692	93% · · ·
1	d	692	92% 5% ·
2	E	20	70% 15% 15%
2	F	20	65% 15% 20%

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Mol	Chain	Length	Quality of chain
2	e	20	
2	f	20	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 26985 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 DNA gyrase subunit B,DNA gyrase subunit B,DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	673	Total	C	N	O	S	0	29	0
			5544	3446	1008	1063	27			
1	D	674	Total	C	N	O	S	0	27	0
			5541	3445	1016	1054	26			
1	b	675	Total	C	N	O	S	0	31	0
			5579	3471	1013	1068	27			
1	d	672	Total	C	N	O	S	0	28	0
			5531	3440	1000	1064	27			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	initiating methionine	UNP P66937
B	544	THR	-	linker	UNP P66937
B	545	GLY	-	linker	UNP P66937
B	1000	ASP	-	linker	UNP P66937
B	1001	PHE	-	linker	UNP P66937
B	1123	PHE	TYR	engineered mutation	UNP Q99XG5
D	409	MET	-	initiating methionine	UNP P66937
D	544	THR	-	linker	UNP P66937
D	545	GLY	-	linker	UNP P66937
D	1000	ASP	-	linker	UNP P66937
D	1001	PHE	-	linker	UNP P66937
D	1123	PHE	TYR	engineered mutation	UNP Q99XG5
b	409	MET	-	initiating methionine	UNP P66937
b	544	THR	-	linker	UNP P66937
b	545	GLY	-	linker	UNP P66937
b	1000	ASP	-	linker	UNP P66937
b	1001	PHE	-	linker	UNP P66937
b	1123	PHE	TYR	engineered mutation	UNP Q99XG5
d	409	MET	-	initiating methionine	UNP P66937
d	544	THR	-	linker	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
d	545	GLY	-	linker	UNP P66937
d	1000	ASP	-	linker	UNP P66937
d	1001	PHE	-	linker	UNP P66937
d	1123	PHE	TYR	engineered mutation	UNP Q99XG5

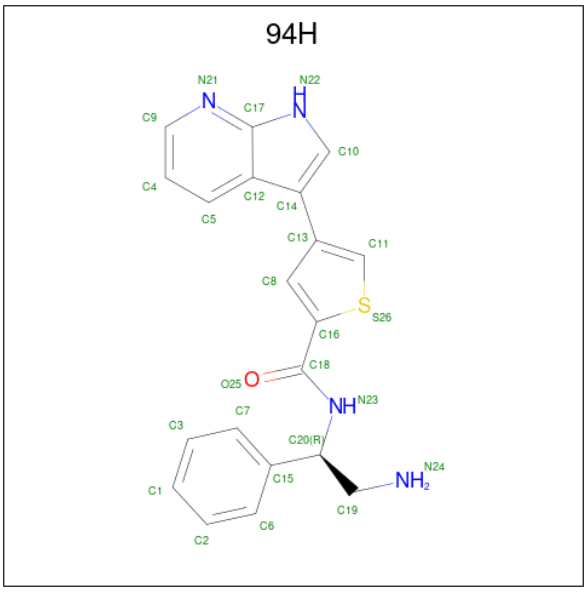
- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	P	0	5	0
			442	212	82	128	20			
2	F	16	Total	C	N	O	P	0	1	0
			345	165	63	101	16			
2	e	20	Total	C	N	O	P	0	5	0
			508	242	94	148	24			
2	f	20	Total	C	N	O	P	0	5	0
			508	242	94	148	24			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

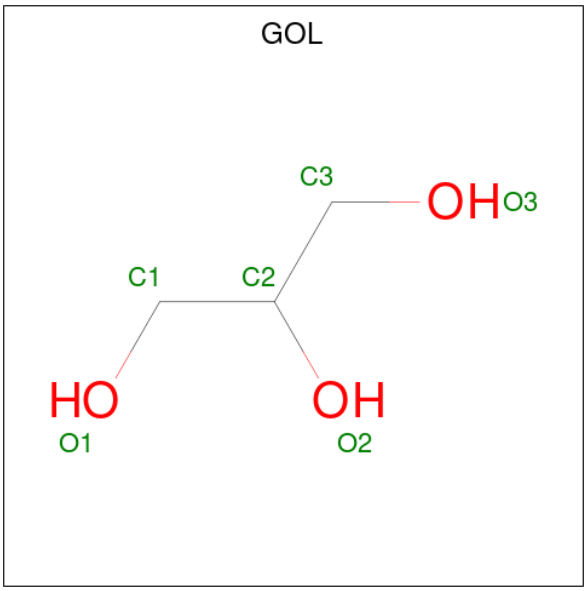
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	b	1	Total	Mn	0	0
			1	1		
3	d	2	Total	Mn	0	0
			2	2		

- Molecule 4 is {N}-[(1 {R})-2-azanyl-1-phenyl-ethyl]-4-(1 {H}-pyrrolo[2,3-b]pyridin-3-yl)thiophene-2-carboxamide (CCD ID: 94H) (formula: $C_{20}H_{18}N_4OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
4	B	1	Total	C	N	O	S	0	1
			26	20	4	1	1		
4	D	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
4	b	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
4	b	1	Total	C	N	O	S	0	1
			26	20	4	1	1		
4	d	1	Total	C	N	O	S	0	0
			26	20	4	1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

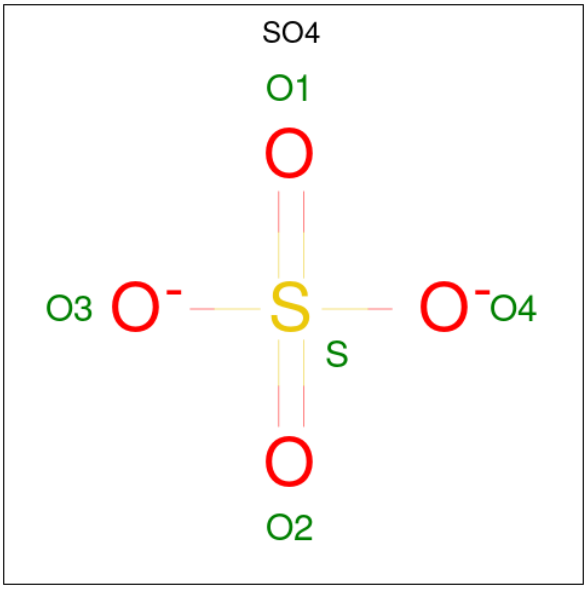


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	b	1	Total	C	O	0	0
			6	3	3		
5	b	1	Total	C	O	0	0
			6	3	3		
5	b	1	Total	C	O	0	0
			6	3	3		
5	d	1	Total	C	O	0	0
			6	3	3		
5	d	1	Total	C	O	0	0
			6	3	3		
5	e	1	Total	C	O	0	1
			12	6	6		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Cl 1 1	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

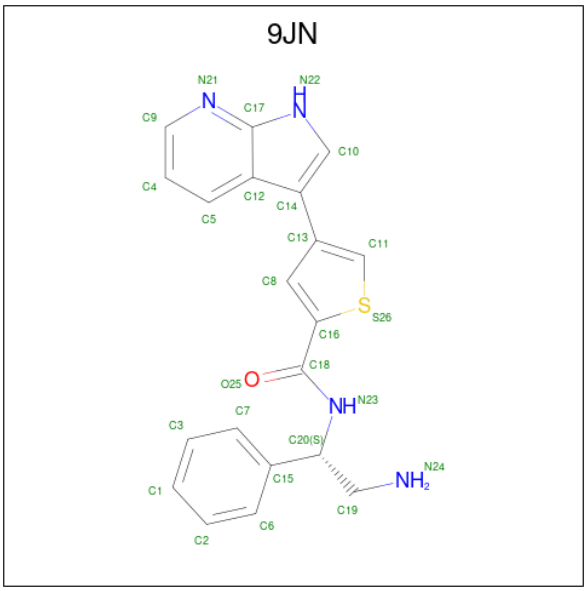


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	b	1	Total O S 5 4 1	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	b	1	Total Na 1 1	0	0

- Molecule 9 is {N}-[(1 {S})-2-azanyl-1-phenyl-ethyl]-4-(1 {H}-pyrrolo[2,3-b]pyridin-3-yl)thiophene-2-carboxamide (CCD ID: 9JN) (formula: $C_{20}H_{18}N_4OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	b	1	Total	C	N	O	S	0	1
			26	20	4	1	1		
9	e	1	Total	C	N	O	S	0	1
			26	20	4	1	1		

- Molecule 10 is water.

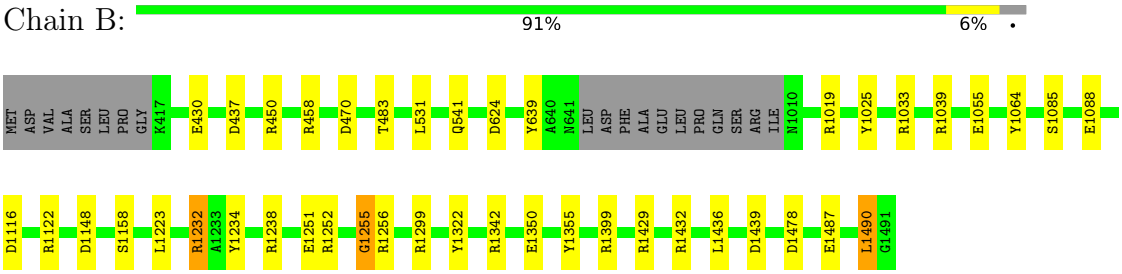
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	617	Total	O	0	3
			620	620		
10	D	599	Total	O	0	3
			602	602		
10	E	56	Total	O	0	4
			60	60		
10	F	60	Total	O	0	1
			61	61		
10	b	612	Total	O	0	2
			614	614		
10	d	606	Total	O	0	4
			610	610		
10	e	65	Total	O	0	1
			66	66		
10	f	49	Total	O	0	1
			50	50		

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.

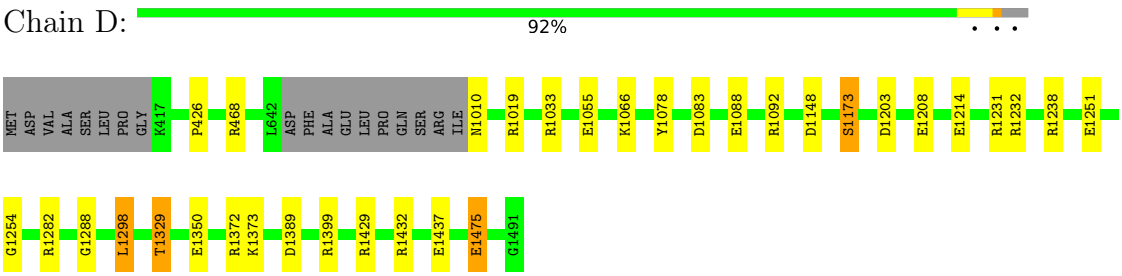
• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B,DNA gyrase subunit A

Chain B:



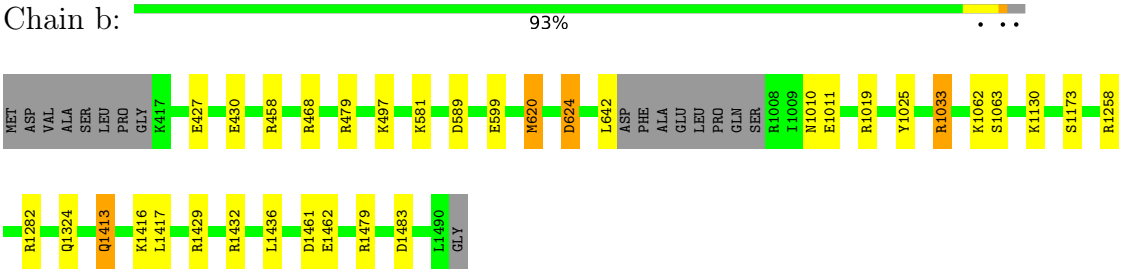
• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B,DNA gyrase subunit A

Chain D:



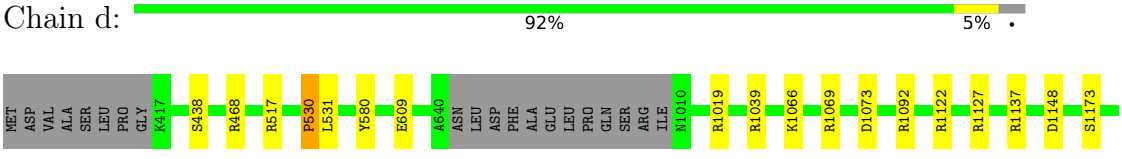
• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B,DNA gyrase subunit A

Chain b:



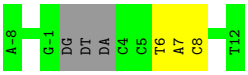
• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B,DNA gyrase subunit A

Chain d:



• Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP *GP*GP*CP*T)-3')

Chain E:

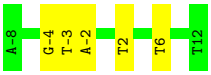


• Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP *GP*GP*CP*T)-3')

Chain F:

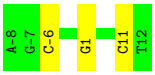
• Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP *GP*GP*CP*T)-3')

Chain e:



• Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP *GP*GP*CP*T)-3')

Chain f:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.44Å 120.68Å 168.90Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	19.97 – 1.98 19.97 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.97-1.98) 98.5 (19.97-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.154 , 0.183 0.153 , 0.178	Depositor DCC
R_{free} test set	12352 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.278 for h,-k,-l	Xtriage
Reported twinning fraction	0.763 for H, K, L 0.237 for h,-k,-l	Depositor
Outliers	0 of 245570 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	26985	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.64% 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: NA, 94H, CL, 9JN, GOL, SO4, MN

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	B	0.96	18/5617 (0.3%)	0.99	36/7565 (0.5%)
1	D	1.05	11/5613 (0.2%)	0.97	30/7555 (0.4%)
1	b	0.98	9/5651 (0.2%)	1.21	22/7608 (0.3%)
1	d	0.95	7/5609 (0.1%)	0.96	31/7557 (0.4%)
2	E	1.02	1/494 (0.2%)	1.13	3/758 (0.4%)
2	F	1.34	3/384 (0.8%)	1.16	1/586 (0.2%)
2	e	1.06	4/568 (0.7%)	1.03	3/872 (0.3%)
2	f	1.09	1/568 (0.2%)	1.27	5/872 (0.6%)
All	All	1.00	54/24504 (0.2%)	1.05	131/33373 (0.4%)

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	B	0	3
1	b	0	1
1	d	0	2
All	All	0	6

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1282[A]	ARG	C-N	-24.07	0.78	1.34
1	D	1282[B]	ARG	C-N	-24.07	0.78	1.34
1	b	479[A]	ARG	C-N	-9.91	1.11	1.34
1	b	479[B]	ARG	C-N	-9.91	1.11	1.34
1	b	1062[A]	LYS	C-N	-9.37	1.12	1.34

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	1413	GLN	O-C-N	-67.37	14.91	122.70
1	B	1232[A]	ARG	NE-CZ-NH1	-12.98	113.81	120.30
1	B	1232[B]	ARG	NE-CZ-NH1	-12.98	113.81	120.30
1	d	1231	ARG	NE-CZ-NH1	-12.96	113.82	120.30
1	d	468	ARG	NE-CZ-NH2	12.19	126.40	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1255	GLY	Mainchain
1	B	639[B]	TYR	Mainchain
1	b	1413	GLN	Mainchain
1	d	530	PRO	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	B	698/692 (101%)	682 (98%)	15 (2%)	1 (0%)	48	41
1	D	698/692 (101%)	678 (97%)	17 (2%)	3 (0%)	30	20
1	b	702/692 (101%)	687 (98%)	14 (2%)	1 (0%)	48	41
1	d	696/692 (101%)	681 (98%)	15 (2%)	0	100	100
All	All	2794/2768 (101%)	2728 (98%)	61 (2%)	5 (0%)	48	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1254[A]	GLY
1	D	1254[B]	GLY
1	B	1033	ARG
1	D	1033	ARG
1	b	1033	ARG

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	B	589/591 (100%)	580 (98%)	9 (2%)	60	56
1	D	589/591 (100%)	573 (97%)	16 (3%)	40	30
1	b	596/591 (101%)	577 (97%)	19 (3%)	34	24
1	d	589/591 (100%)	579 (98%)	10 (2%)	56	49
All	All	2363/2364 (100%)	2309 (98%)	54 (2%)	56	38

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	468[A]	ARG
1	b	620[B]	MET
1	d	1276[A]	LYS
1	b	468[B]	ARG
1	b	581[A]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1412	GLN
1	b	476	ASN
1	b	480	GLN
1	d	1324	GLN
1	d	1412	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 7 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	d	1503	-	5,5,5	0.36	0	5,5,5	0.79	0
5	GOL	e	102[B]	-	5,5,5	0.35	0	5,5,5	0.99	0
4	94H	D	1503	-	24,29,29	1.60	6 (25%)	26,40,40	1.98	5 (19%)
5	GOL	B	1505	-	5,5,5	0.32	0	5,5,5	0.92	0
5	GOL	D	1505	-	5,5,5	0.90	0	5,5,5	0.43	0
5	GOL	D	1502	-	5,5,5	0.42	0	5,5,5	0.75	0
4	94H	b	1509[B]	-	24,29,29	1.24	2 (8%)	26,40,40	1.64	3 (11%)
4	94H	b	1502	-	24,29,29	1.47	4 (16%)	26,40,40	1.91	6 (23%)
7	SO4	b	1506	-	4,4,4	0.28	0	6,6,6	0.88	0
5	GOL	b	1503	-	5,5,5	0.44	0	5,5,5	0.41	0
5	GOL	D	1506	-	5,5,5	0.52	0	5,5,5	0.63	0
9	9JN	e	101[B]	-	24,29,29	1.16	2 (8%)	26,40,40	2.35	7 (26%)
9	9JN	b	1508[A]	-	24,29,29	1.24	4 (16%)	26,40,40	2.32	9 (34%)
5	GOL	B	1504	-	5,5,5	0.55	0	5,5,5	0.67	0
5	GOL	B	1503	-	5,5,5	0.82	0	5,5,5	0.37	0
5	GOL	D	1504	-	5,5,5	0.52	0	5,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	94H	B	1506[A]	-	24,29,29	1.29	2 (8%)	26,40,40	1.85	6 (23%)
4	94H	d	1502	-	24,29,29	1.36	4 (16%)	26,40,40	1.62	3 (11%)
4	94H	B	1502	-	24,29,29	1.43	3 (12%)	26,40,40	1.43	2 (7%)
5	GOL	e	102[A]	-	5,5,5	0.46	0	5,5,5	0.50	0
5	GOL	d	1504	-	5,5,5	0.79	0	5,5,5	0.43	0
5	GOL	b	1504	-	5,5,5	0.63	0	5,5,5	0.61	0
5	GOL	b	1505	-	5,5,5	0.53	0	5,5,5	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	d	1503	-	-	0/4/4/4	-
5	GOL	e	102[B]	-	-	3/4/4/4	-
4	94H	D	1503	-	-	3/14/18/18	0/4/4/4
5	GOL	B	1505	-	-	4/4/4/4	-
5	GOL	D	1505	-	-	0/4/4/4	-
5	GOL	D	1502	-	-	3/4/4/4	-
4	94H	b	1509[B]	-	-	8/14/18/18	0/4/4/4
4	94H	b	1502	-	-	4/14/18/18	0/4/4/4
5	GOL	b	1503	-	-	2/4/4/4	-
5	GOL	D	1506	-	-	3/4/4/4	-
9	9JN	e	101[B]	-	-	3/14/18/18	0/4/4/4
9	9JN	b	1508[A]	-	-	4/14/18/18	0/4/4/4
5	GOL	B	1504	-	-	4/4/4/4	-
5	GOL	B	1503	-	-	2/4/4/4	-
5	GOL	D	1504	-	-	0/4/4/4	-
4	94H	B	1506[A]	-	-	7/14/18/18	0/4/4/4
4	94H	d	1502	-	-	3/14/18/18	0/4/4/4
4	94H	B	1502	-	-	4/14/18/18	0/4/4/4
5	GOL	e	102[A]	-	-	2/4/4/4	-
5	GOL	d	1504	-	-	3/4/4/4	-
5	GOL	b	1504	-	-	0/4/4/4	-
5	GOL	b	1505	-	-	2/4/4/4	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	1502	94H	C17-N21	-4.14	1.31	1.37
4	D	1503	94H	C14-C13	-3.99	1.42	1.49
4	D	1503	94H	C17-N21	-3.55	1.32	1.37
9	b	1508[A]	9JN	C14-C13	-3.54	1.43	1.49
4	B	1502	94H	C16-S26	-3.52	1.68	1.72

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	b	1508[A]	9JN	C9-N21-C17	-5.30	110.07	116.60
9	e	101[B]	9JN	C20-N23-C18	5.21	129.05	122.34
4	D	1503	94H	C20-N23-C18	-5.04	115.84	122.34
4	b	1502	94H	C9-N21-C17	-5.04	110.39	116.60
4	D	1503	94H	C9-N21-C17	-5.01	110.42	116.60

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

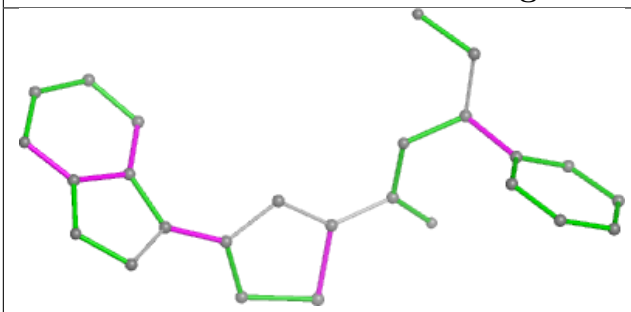
Mol	Chain	Res	Type	Atoms
4	B	1502	94H	C8-C13-C14-C10
4	B	1502	94H	C11-C13-C14-C10
4	B	1506[A]	94H	C8-C16-C18-N23
4	B	1506[A]	94H	C8-C16-C18-O25
4	D	1503	94H	C8-C13-C14-C10

There are no ring outliers.

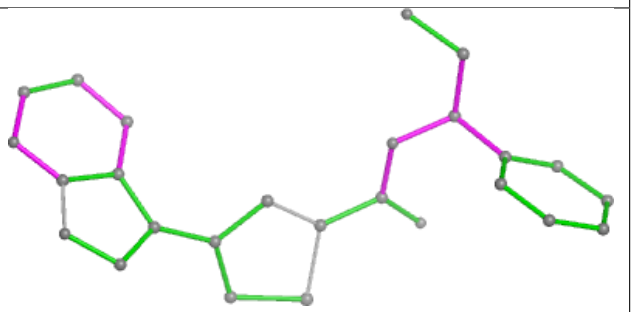
No monomer is involved in short contacts.

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 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.

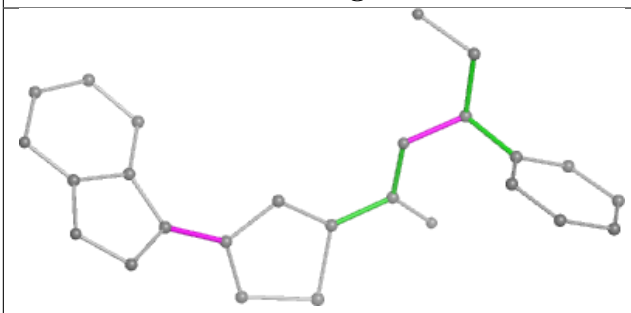
Ligand 94H D 1503



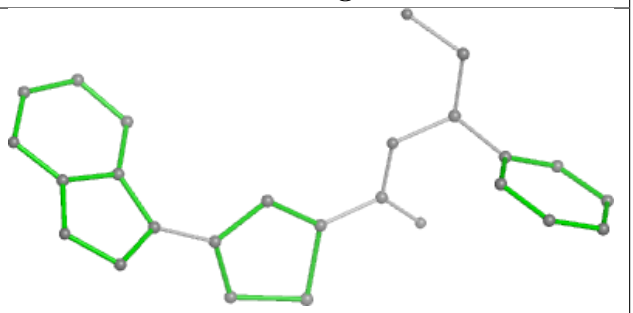
Bond lengths



Bond angles

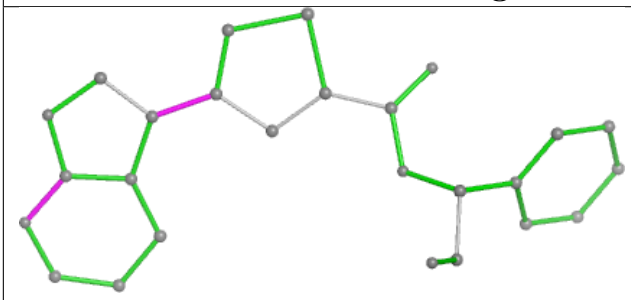


Torsions

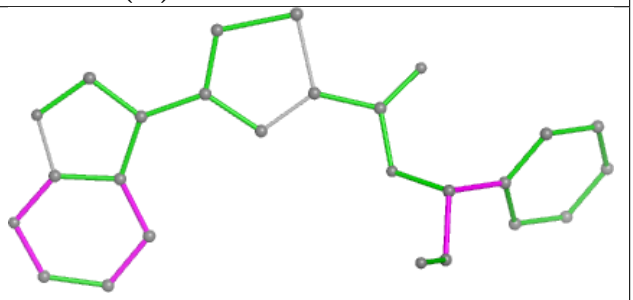


Rings

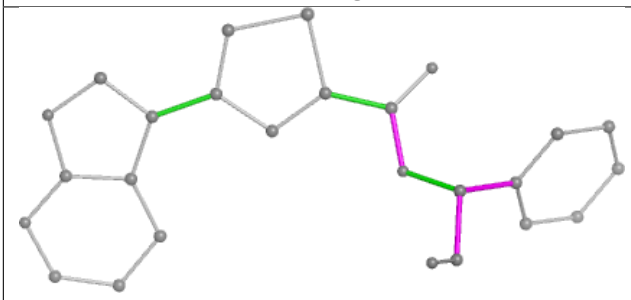
Ligand 94H b 1509 (B)



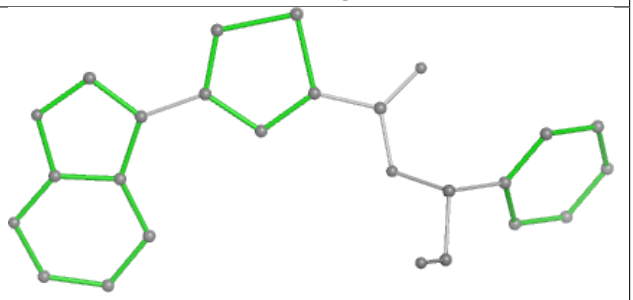
Bond lengths



Bond angles

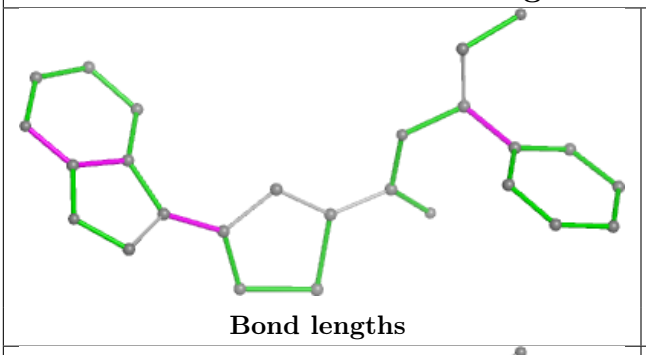


Torsions

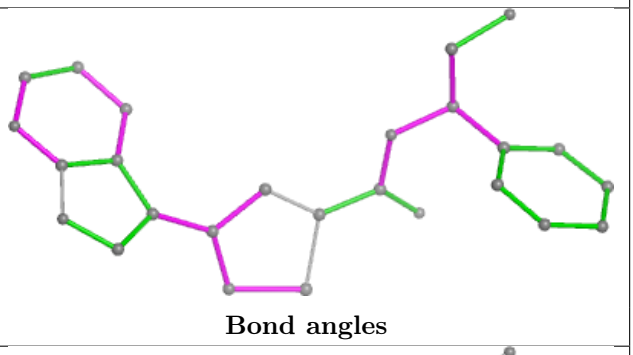


Rings

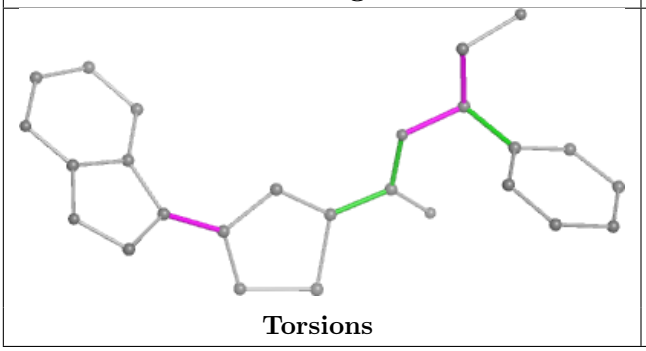
Ligand 94H b 1502



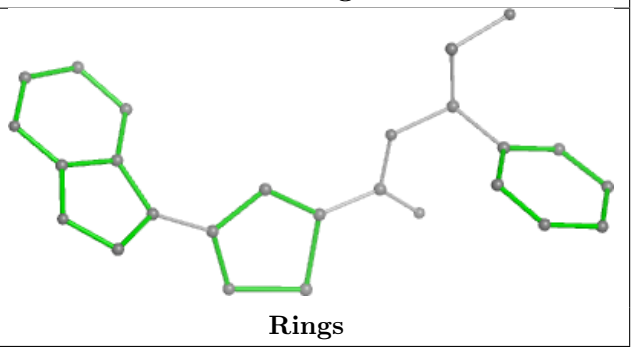
Bond lengths



Bond angles

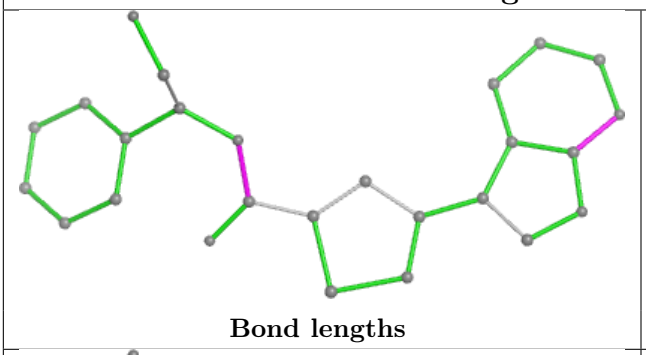


Torsions

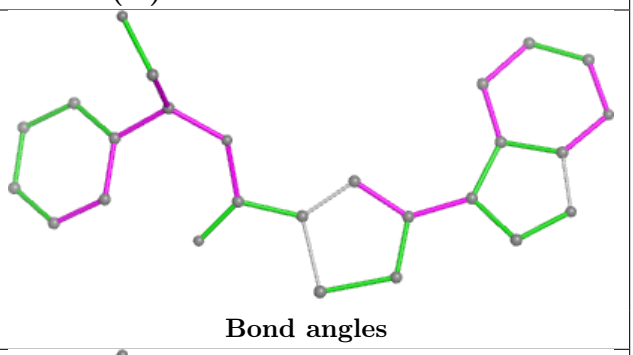


Rings

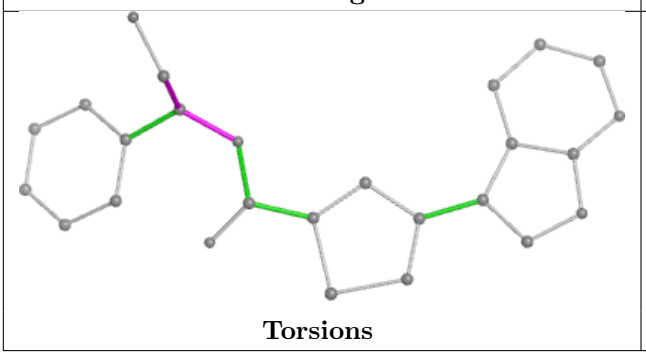
Ligand 9JN e 101 (B)



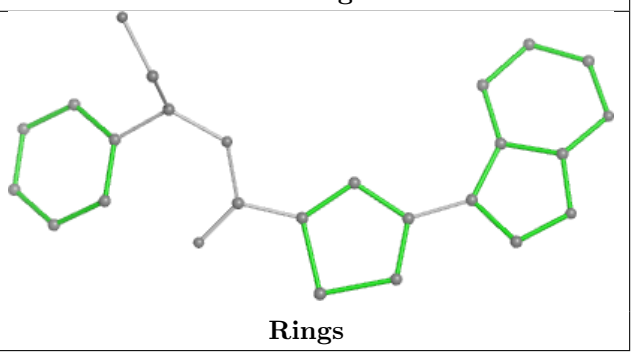
Bond lengths



Bond angles

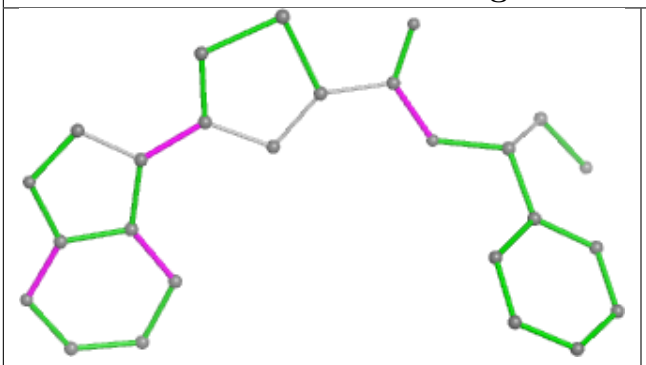


Torsions

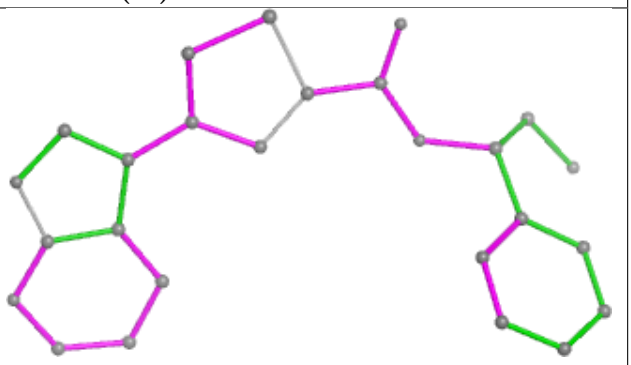


Rings

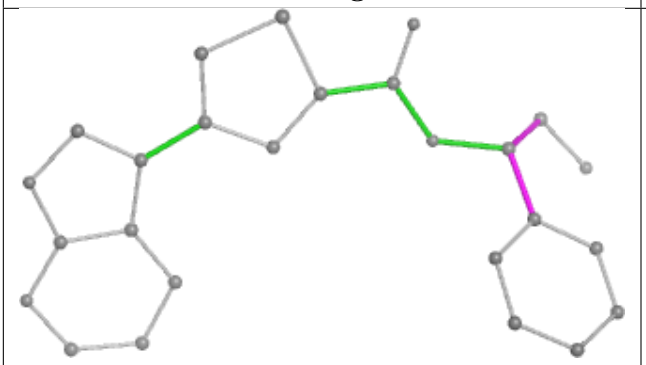
Ligand 9JN b 1508 (A)



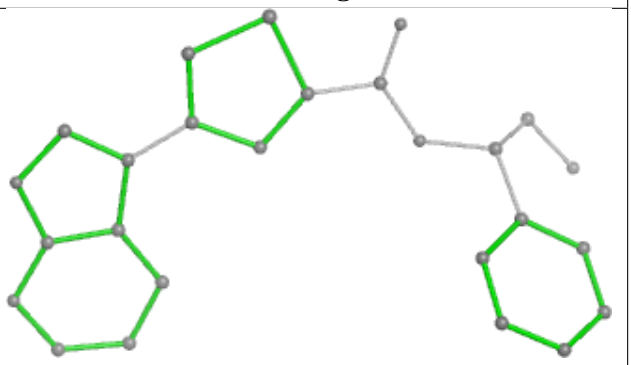
Bond lengths



Bond angles

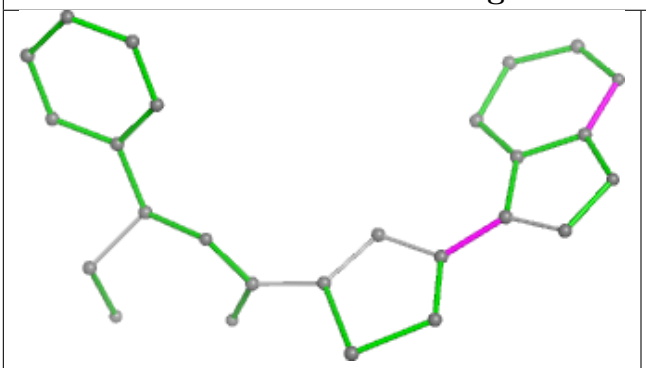


Torsions

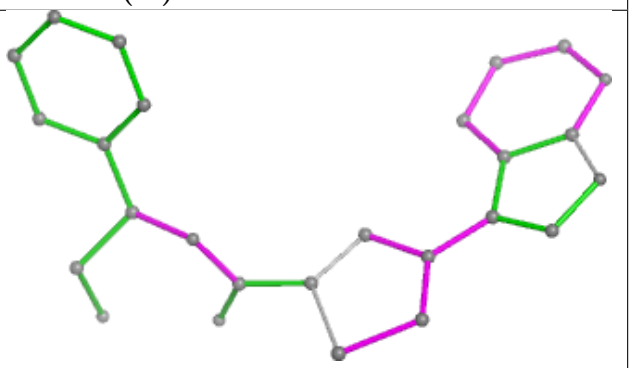


Rings

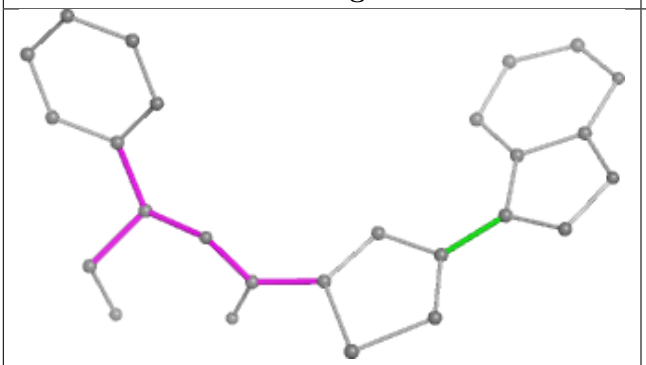
Ligand 94H B 1506 (A)



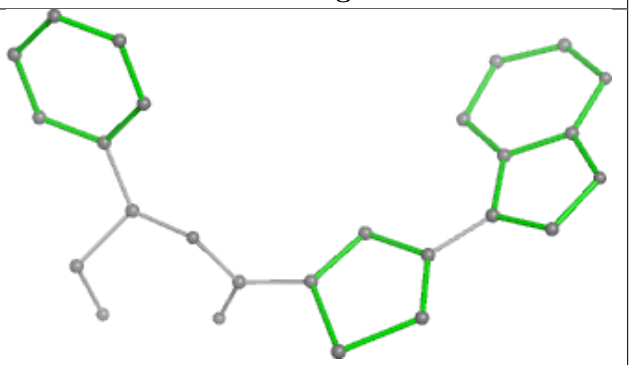
Bond lengths



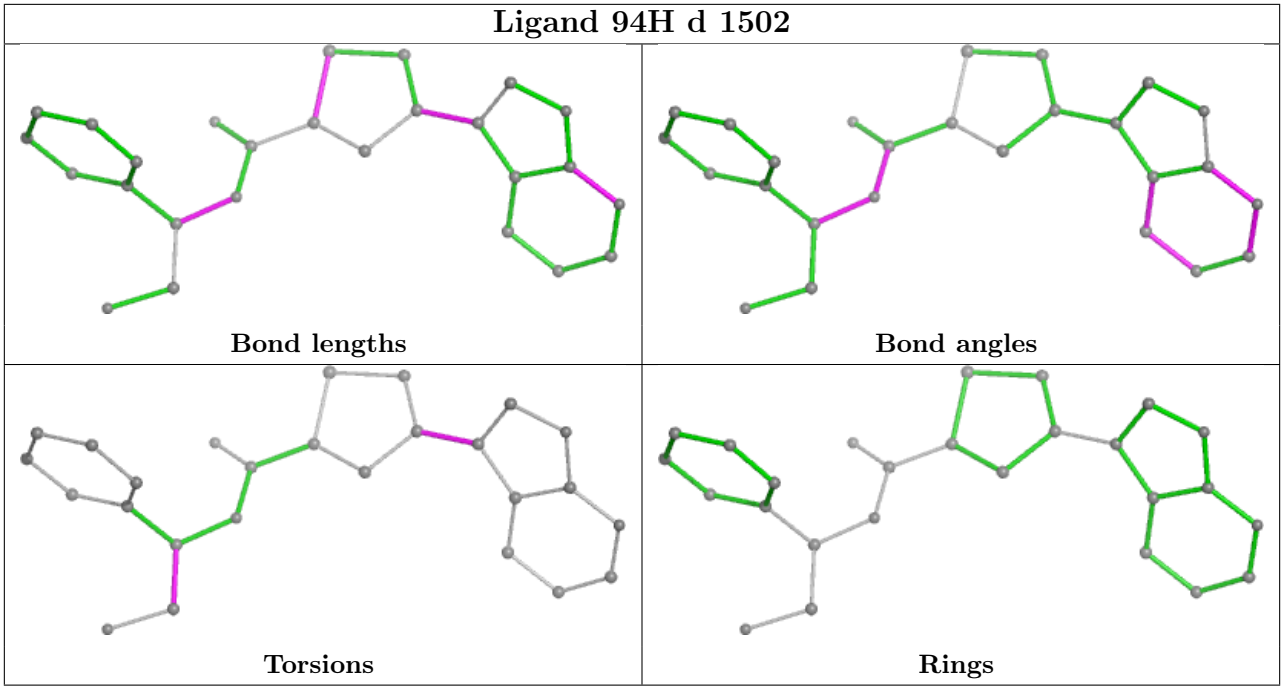
Bond angles

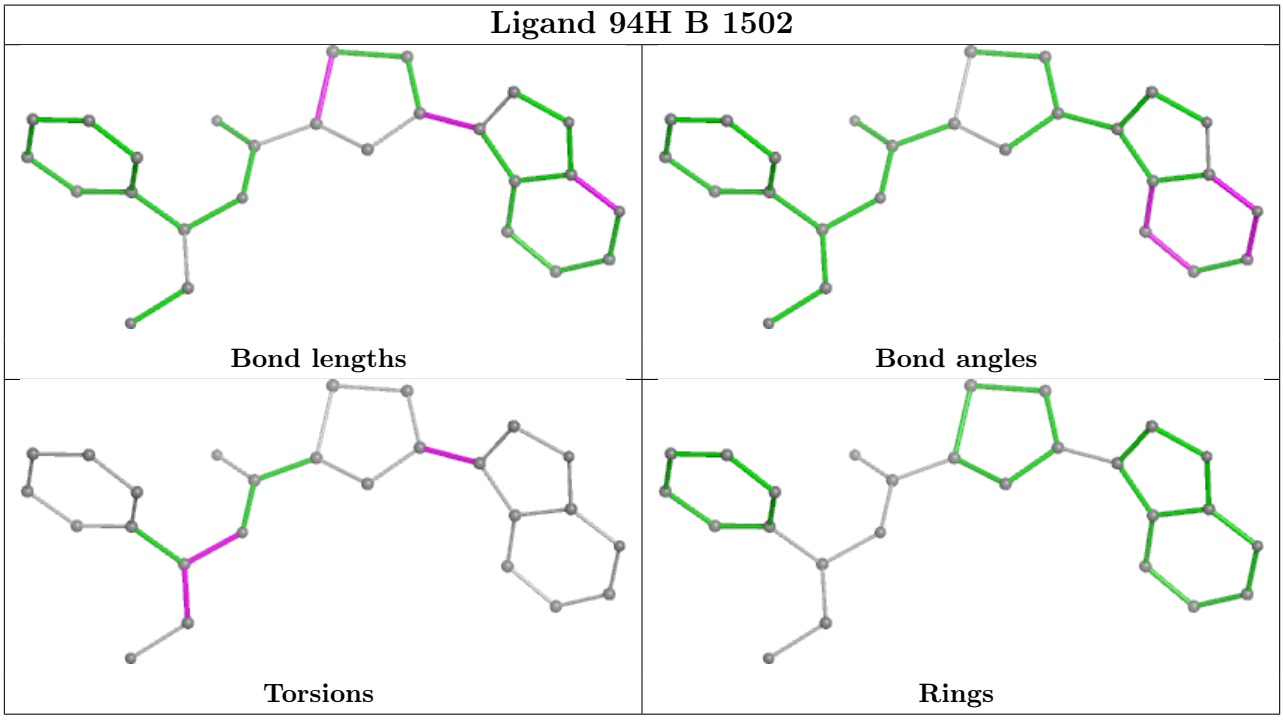


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	b	5
2	e	2
2	f	2
1	d	2
1	D	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	-1:DG	O3'	1[B]:DG	P	9.96
1	f	-1:DG	O3'	1[A]:DG	P	7.59
1	e	-1:DG	O3'	1[A]:DG	P	6.98
1	f	-1:DG	O3'	1[B]:DG	P	5.32
1	b	1413:GLN	C	1414[A]:ARG	N	1.19

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^{th} 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	B	673/692 (97%)	-1.52	0	100	100	11, 32, 54, 83	29 (4%)
1	D	674/692 (97%)	-1.50	0	100	100	8, 33, 59, 85	27 (4%)
1	b	675/692 (97%)	-1.50	0	100	100	11, 32, 62, 94	31 (4%)
1	d	672/692 (97%)	-1.50	0	100	100	13, 33, 55, 73	28 (4%)
2	E	17/20 (85%)	-1.45	0	100	100	17, 26, 42, 47	6 (35%)
2	F	16/20 (80%)	-1.67	0	100	100	23, 27, 46, 50	1 (6%)
2	e	20/20 (100%)	-1.23	0	100	100	21, 34, 72, 88	5 (25%)
2	f	20/20 (100%)	-1.33	0	100	100	23, 30, 60, 63	5 (25%)
All	All	2767/2848 (97%)	-1.50	0	100	100	8, 32, 58, 94	132 (4%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

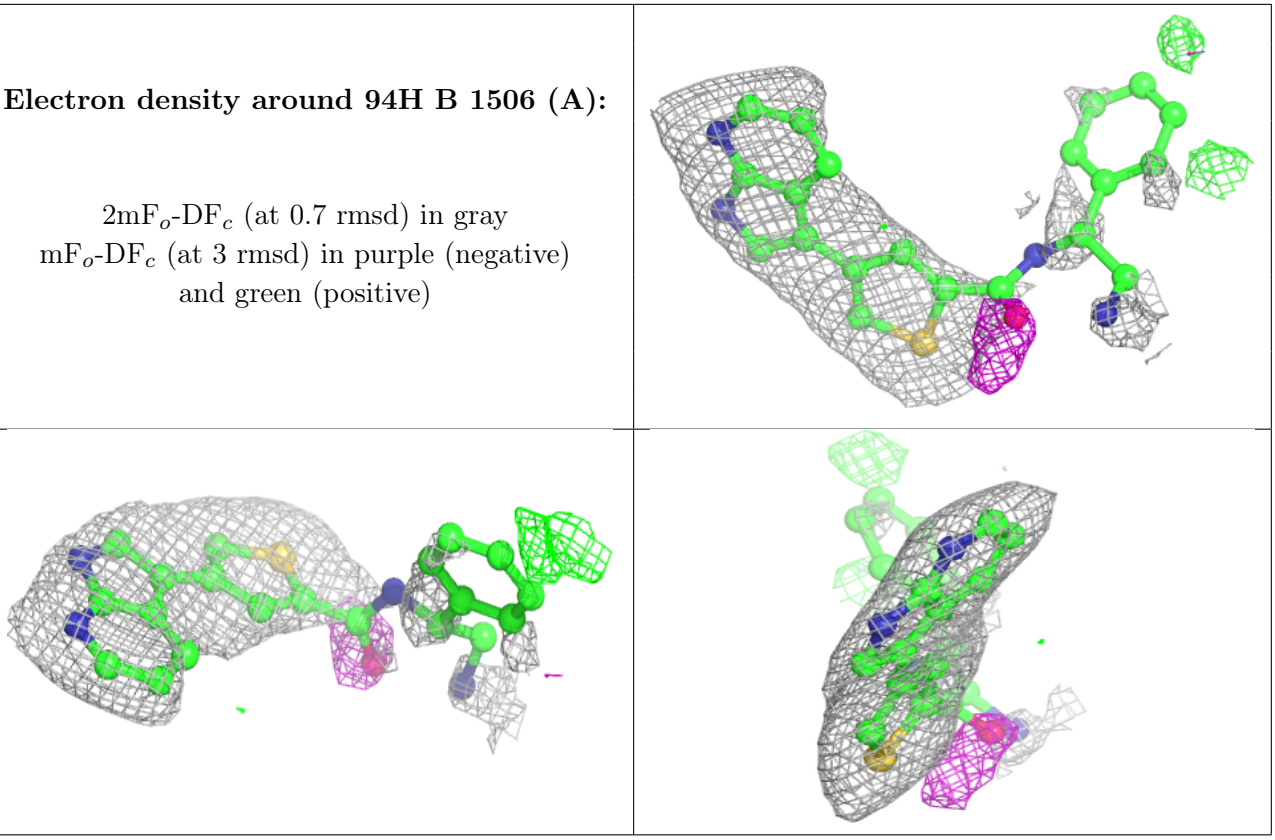
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	94H	B	1506[A]	26/26	0.96	0.09	38,48,64,66	26
5	GOL	D	1502	6/6	0.97	0.05	52,54,55,60	0
5	GOL	D	1506	6/6	0.97	0.05	43,52,57,58	0
9	9JN	b	1508[A]	26/26	0.97	0.07	35,43,48,54	26
9	9JN	e	101[B]	26/26	0.97	0.07	29,48,60,68	26
5	GOL	b	1505	6/6	0.98	0.06	39,47,58,64	0
5	GOL	d	1503	6/6	0.98	0.04	48,54,58,63	0
5	GOL	e	102[A]	6/6	0.98	0.06	33,37,42,43	6
5	GOL	e	102[B]	6/6	0.98	0.06	29,33,35,36	6
7	SO4	b	1506	5/5	0.98	0.03	38,45,48,48	5
4	94H	b	1509[B]	26/26	0.98	0.09	50,75,107,109	26
5	GOL	B	1504	6/6	0.98	0.04	52,55,57,65	0
5	GOL	b	1504	6/6	0.99	0.03	25,38,39,43	0
3	MN	d	1505	1/1	0.99	0.03	84,84,84,84	0
5	GOL	B	1505	6/6	0.99	0.04	53,61,65,65	0
5	GOL	d	1504	6/6	0.99	0.03	35,39,51,54	0
4	94H	d	1502	26/26	0.99	0.03	28,40,51,53	0
5	GOL	D	1504	6/6	0.99	0.03	32,41,47,51	0
6	CL	D	1507	1/1	0.99	0.04	41,41,41,41	1
5	GOL	D	1505	6/6	0.99	0.03	26,34,41,45	0
8	NA	b	1507	1/1	0.99	0.06	47,47,47,47	0
5	GOL	B	1503	6/6	0.99	0.05	50,57,59,65	0
5	GOL	b	1503	6/6	0.99	0.05	36,41,47,48	0
3	MN	b	1501	1/1	1.00	0.01	24,24,24,24	0
3	MN	d	1501	1/1	1.00	0.01	27,27,27,27	0
3	MN	B	1501	1/1	1.00	0.00	25,25,25,25	0
4	94H	B	1502	26/26	1.00	0.02	22,26,30,32	0
3	MN	D	1501	1/1	1.00	0.01	27,27,27,27	0
4	94H	D	1503	26/26	1.00	0.02	27,35,46,56	0
4	94H	b	1502	26/26	1.00	0.02	18,25,30,32	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.

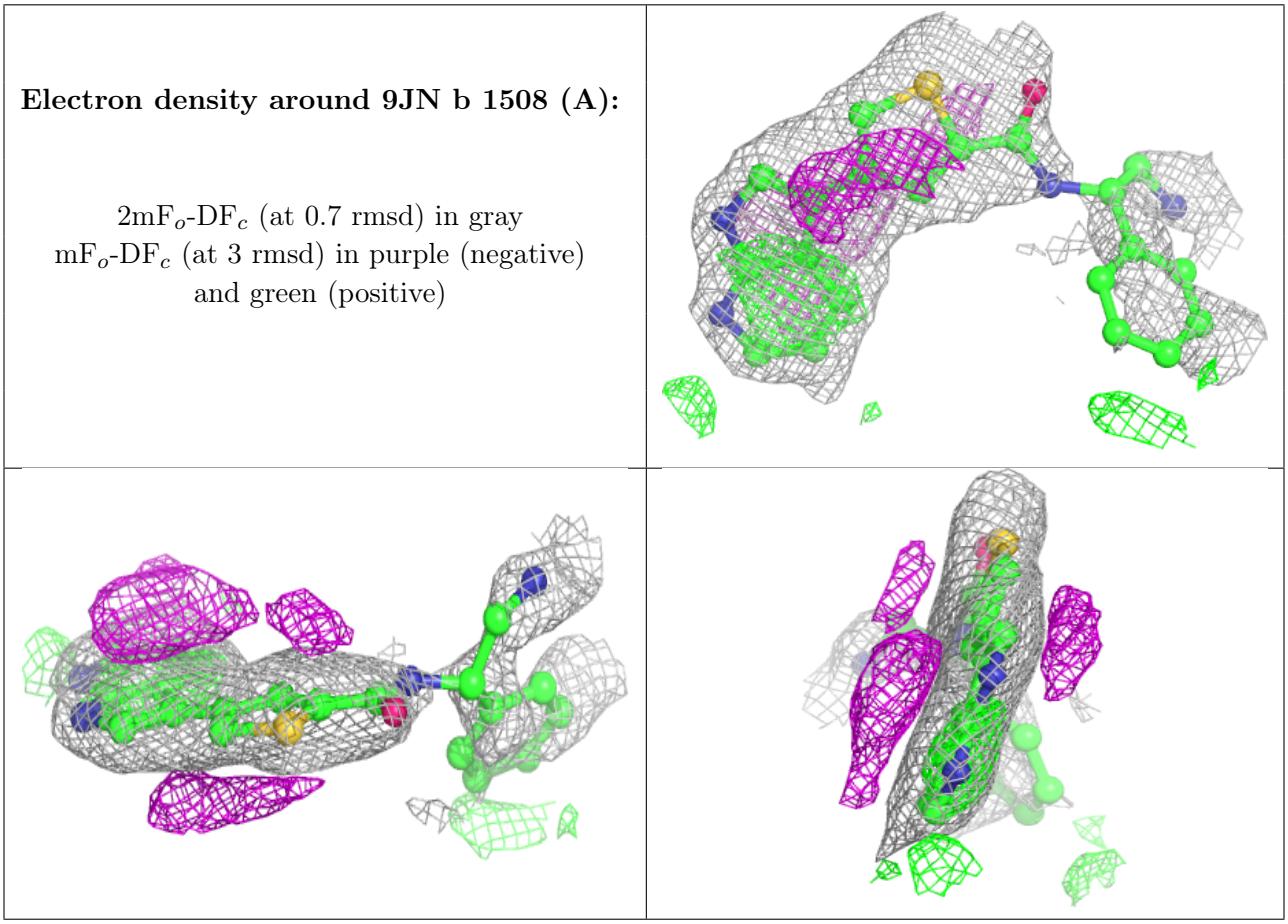
Electron density around 94H B 1506 (A):

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



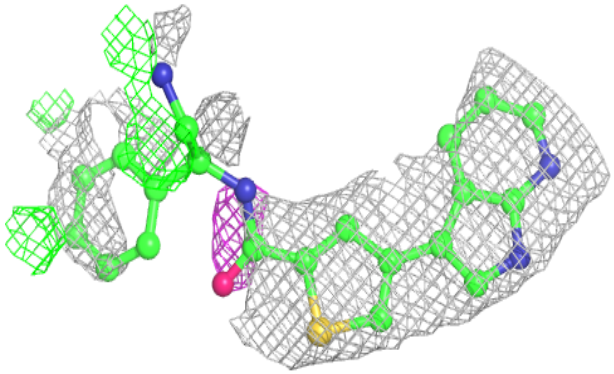
Electron density around 9JN b 1508 (A):

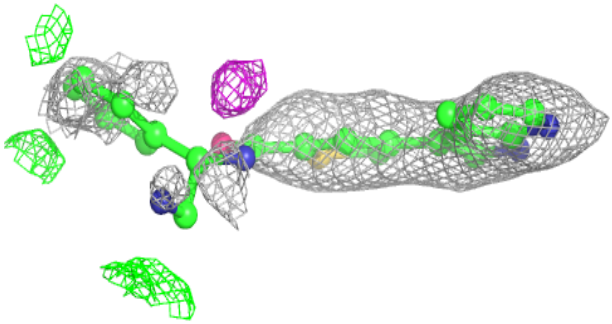
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

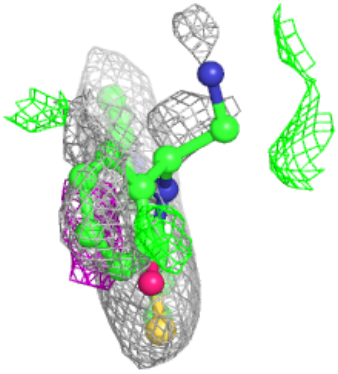


Electron density around 9JN e 101 (B):

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

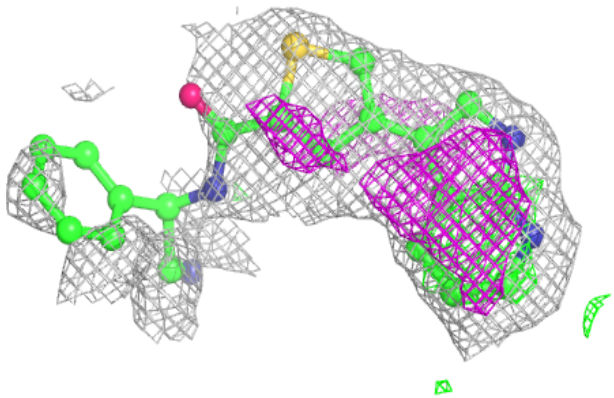


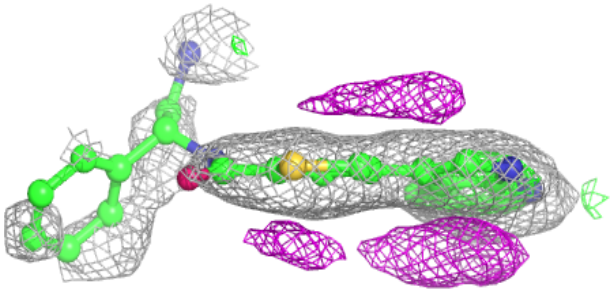


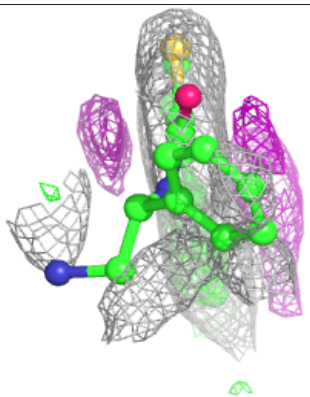


Electron density around 94H b 1509 (B):

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

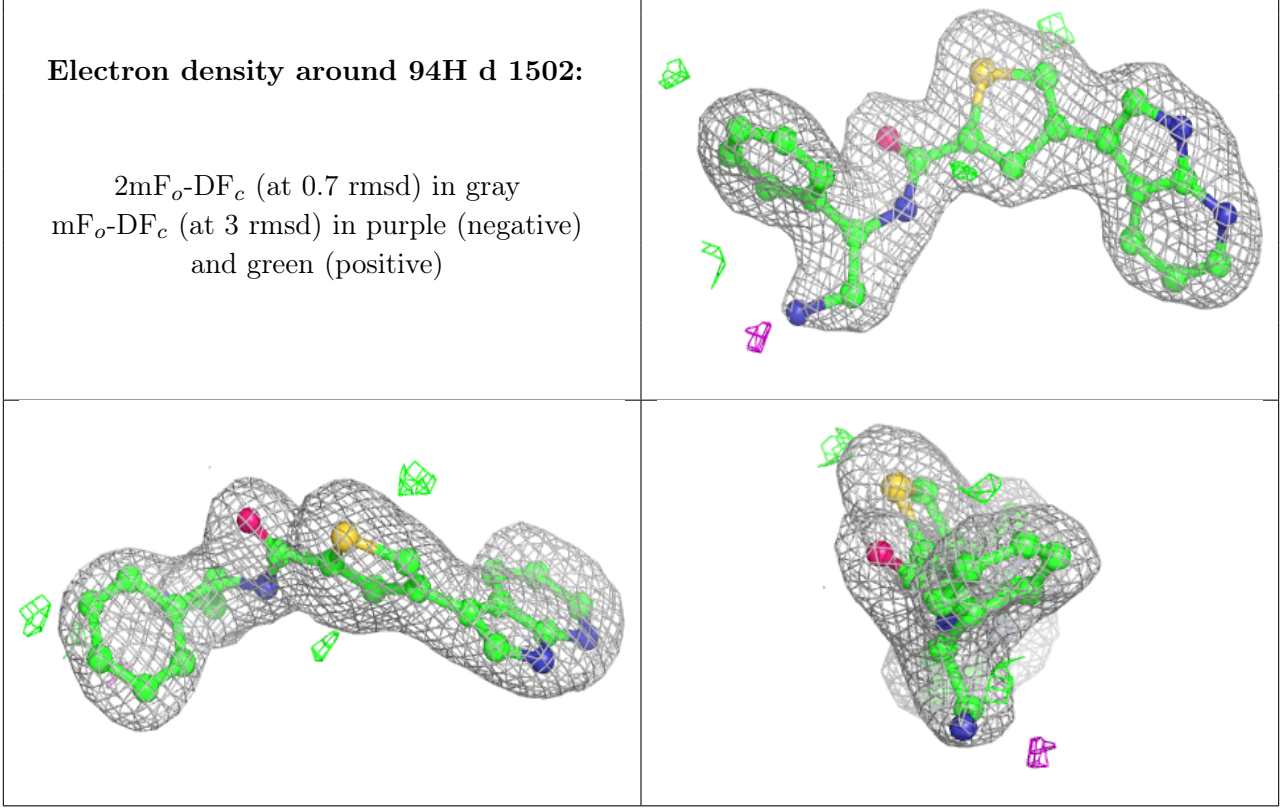






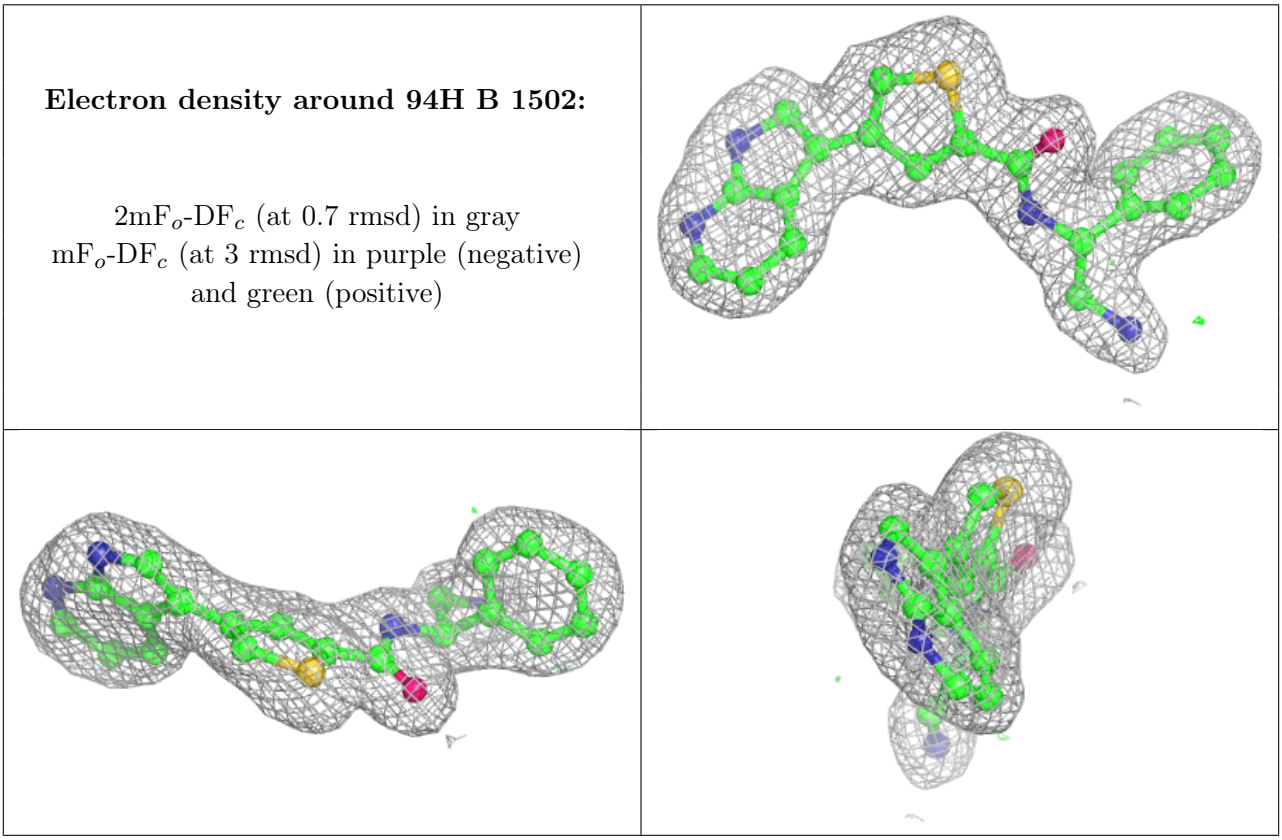
Electron density around 94H d 1502:

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



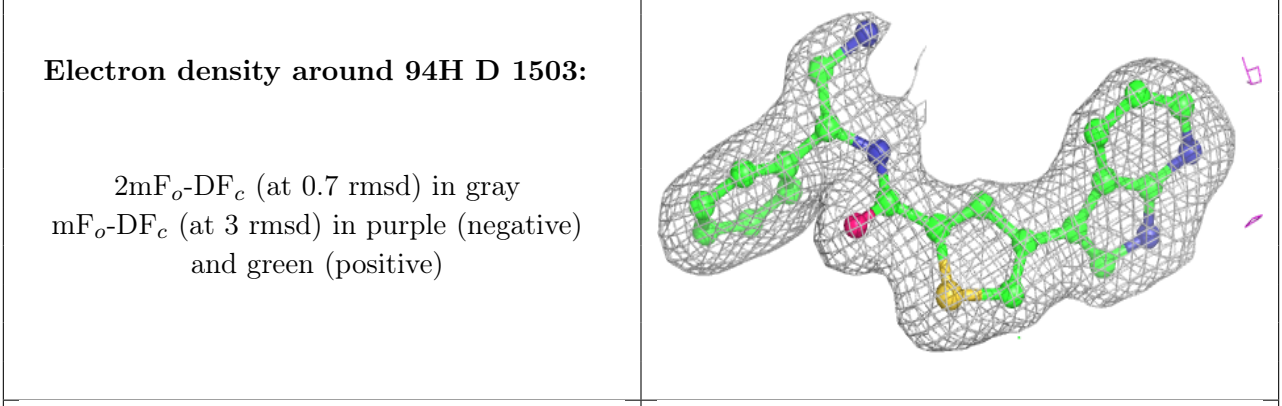
Electron density around 94H B 1502:

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



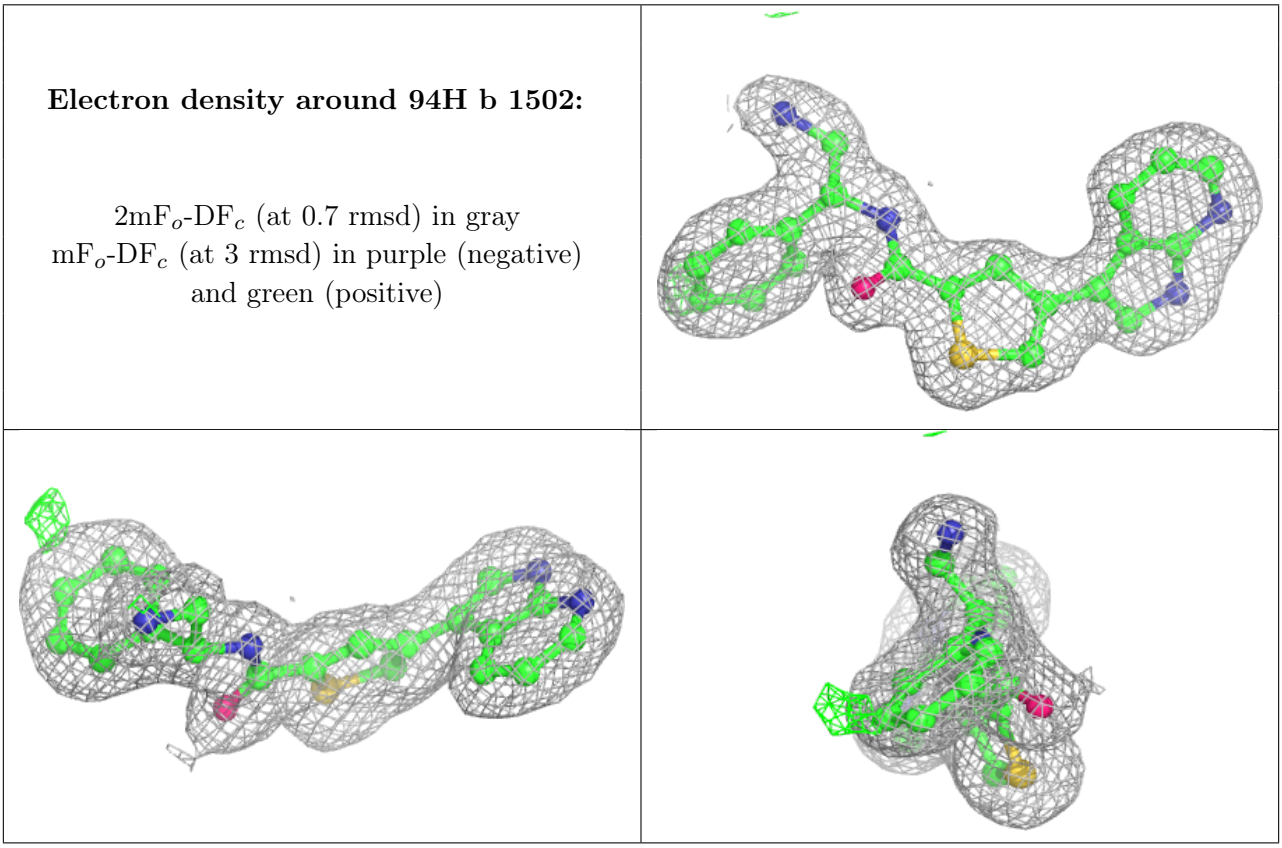
Electron density around 94H D 1503:

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



Electron density around 94H b 1502:

$2mF_o$-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.