



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:14 PM UTC

PDB ID : 5NPP / pdb_00005npp
Title : 2.22A STRUCTURE OF THIOPHENE2 AND GSK945237 WITH S.AUREUS
DNA GYRASE AND DNA
Authors : Bax, B.D.; Chan, P.F.; Stavenger, R.A.
Deposited on : 2017-04-18
Resolution : 2.22 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

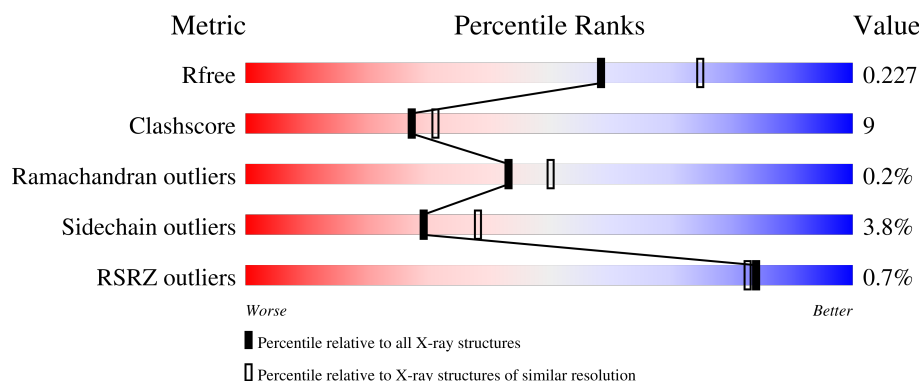
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 $\leq 5\%$. 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	B	692	% 81% 14% ..
1	D	692	% 79% 15% ..
2	E	8	62% 38%
2	F	8	62% 12% 25%
3	A	12	75% 25%

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Mol	Chain	Length	Quality of chain
3	C	12	 A horizontal bar chart showing the quality of chain C. The bar is divided into three segments: green (58%), yellow (33%), and orange (8%).

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12913 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	672	Total	C	N	O	S	0	28	0
			5536	3444	998	1067	27			
1	D	671	Total	C	N	O	S	0	14	0
			5411	3366	975	1043	27			

There are 10 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
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

- 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	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			
2	F	8	Total	C	N	O	P	0	1	0
			181	88	38	48	7			

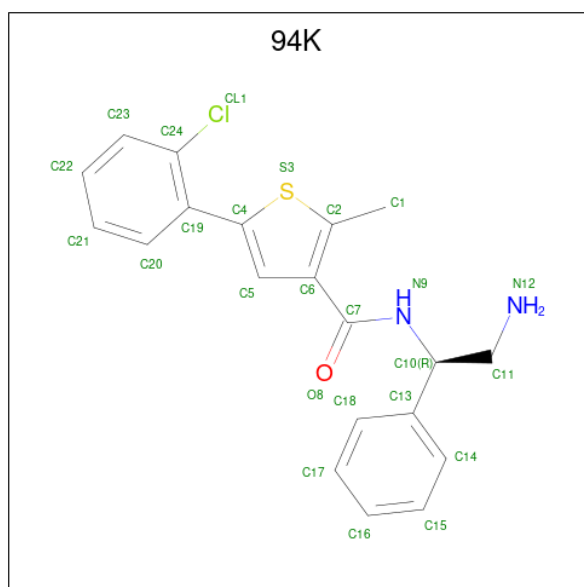
- Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	12	Total	C	N	O	P	0	4	0
			324	154	56	98	16			
3	C	12	Total	C	N	O	P	0	3	0
			270	124	47	84	15			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		

- Molecule 5 is {N}-[(1 {R})-2-azanyl-1-phenyl-ethyl]-5-(2-chlorophenyl)-2-methyl-thiophene-3-carboxamide (CCD ID: 94K) (formula: C₂₀H₁₉ClN₂OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	S	0	0
			25	20	1	2	1	1		
5	D	1	Total	C	Cl	N	O	S	0	0
			25	20	1	2	1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

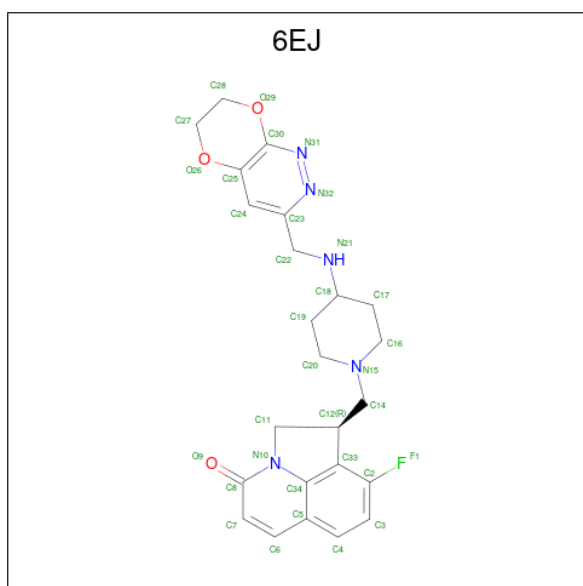
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		

- Molecule 8 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 9 is (1R)-1-[(4-{[(6,7-dihydro[1,4]dioxino[2,3-c]pyridazin-3-yl)methyl]amino}piperidin-1-yl)methyl]-9-fluoro-1,2-dihydro-4H-pyrrolo[3,2,1-ij]quinolin-4-one (CCD ID: 6EJ) (formula: $C_{24}H_{26}FN_5O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	F	N	O	0	1
			66	48	2	10	6		

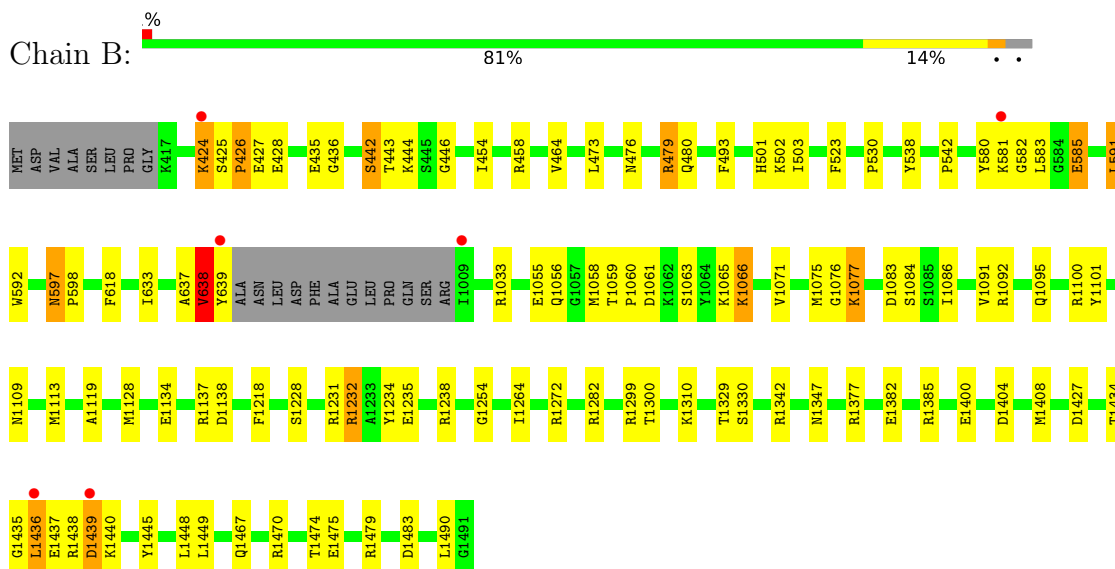
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	394	Total 399	O 399	0	5
10	D	366	Total 368	O 368	0	2
10	E	13	Total 13	O 13	0	0
10	A	27	Total 28	O 28	0	1
10	F	18	Total 18	O 18	0	0
10	C	25	Total 25	O 25	0	0

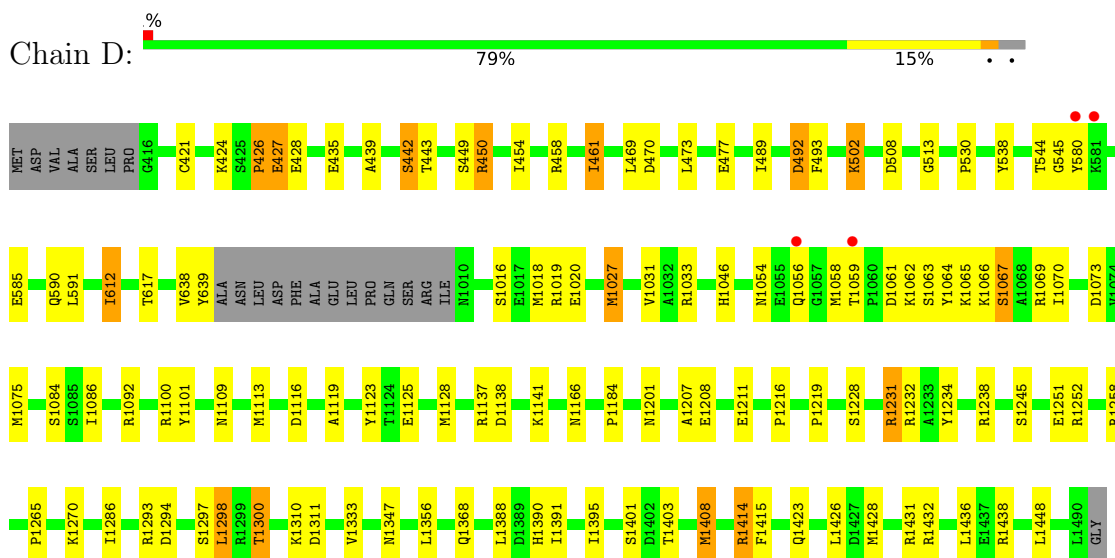
3 Residue-property plots [i](#)

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



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



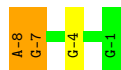
- Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')

Chain E:  62% 38%



- 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:  62% 12% 25%



- Molecule 3: 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 A:  75% 25%



- Molecule 3: 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 C:  58% 33% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	92.85Å 92.85Å 409.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.22 19.89 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.89-2.22) 99.1 (19.89-2.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.182 , 0.227 0.182 , 0.227	Depositor DCC
R_{free} test set	4893 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12913	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: DMS, GOL, 94K, NA, 6EJ, 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	1.05	7/5609 (0.1%)	1.09	11/7554 (0.1%)
1	D	1.06	4/5483 (0.1%)	1.08	13/7389 (0.2%)
2	E	0.55	0/183	0.99	1/281 (0.4%)
2	F	0.80	1/204 (0.5%)	1.84	9/314 (2.9%)
3	A	0.47	0/361	0.82	1/554 (0.2%)
3	C	0.52	0/299	1.12	6/457 (1.3%)
All	All	1.02	12/12139 (0.1%)	1.10	41/16549 (0.2%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1231	ARG	C-O	-7.42	1.15	1.24
2	F	-7	DG	P-OP2	-7.40	1.33	1.48
1	B	428	GLU	N-CA	-7.33	1.37	1.46
1	B	426	PRO	C-O	-6.73	1.15	1.24
1	B	1474	THR	C-O	-5.92	1.17	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	-7	DG	O5'-P-OP1	-11.48	74.56	109.00
2	F	-8[A]	DA	C4'-C3'-O3'	11.22	126.84	110.00
2	F	-8[B]	DA	C4'-C3'-O3'	11.22	126.84	110.00
2	F	-8[A]	DA	C2'-C3'-O3'	-10.32	96.02	111.50
2	F	-8[B]	DA	C2'-C3'-O3'	-10.32	96.02	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5536	0	5509	106	0
1	D	5411	0	5394	99	0
2	E	163	0	91	3	0
2	F	181	0	103	5	0
3	A	324	0	181	6	0
3	C	270	0	145	4	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	25	0	0	1	0
5	D	25	0	0	1	0
6	A	6	0	8	3	0
6	B	18	0	24	2	0
6	C	6	0	8	3	0
6	D	24	0	32	2	0
7	B	1	0	0	0	0
8	B	4	0	6	2	0
9	C	66	0	0	0	0
10	A	28	0	0	1	0
10	B	399	0	0	16	2
10	C	25	0	0	4	0
10	D	368	0	0	12	2
10	E	13	0	0	1	0
10	F	18	0	0	1	0
All	All	12913	0	11501	215	2

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 9.

The worst 5 of 215 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:CG2	1:B:454:ILE:HD12	1.86	1.06
1:D:443[B]:THR:HG22	1:D:591:LEU:HD21	1.36	1.02
2:E:-1:DG:H2''	3:A:1[A]:DG:H5'	1.41	1.02
1:D:1138:ASP:OD1	1:D:1141:LYS:NZ	1.93	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:HG22	1:B:454:ILE:HD12	1.44	0.97

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1921:HOH:O	10:D:1950:HOH:O[5_554]	2.14	0.06
10:B:1917:HOH:O	10:D:1938:HOH:O[1_655]	2.17	0.03

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	695/692 (100%)	673 (97%)	19 (3%)	3 (0%)	30 33
1	D	681/692 (98%)	668 (98%)	12 (2%)	1 (0%)	48 56
All	All	1376/1384 (99%)	1341 (98%)	31 (2%)	4 (0%)	43 41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1033	ARG
1	D	1033	ARG
1	B	638[A]	VAL
1	B	638[B]	VAL

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	590/591 (100%)	567 (96%)	23 (4%)	28	37
1	D	579/591 (98%)	553 (96%)	26 (4%)	24	31
All	All	1169/1182 (99%)	1120 (96%)	49 (4%)	29	34

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	489	ILE
1	D	1031	VAL
1	D	492	ASP
1	D	612	ILE
1	D	1228	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	501	HIS
1	D	590	GLN
1	D	1368	GLN
1	D	1334	ASN
1	B	1010	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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
6	GOL	C	102	-	5,5,5	0.81	0	5,5,5	0.93	0
9	6EJ	C	101[A]	-	36,38,38	1.27	4 (11%)	46,55,55	1.67	9 (19%)
6	GOL	B	1503	-	5,5,5	0.67	0	5,5,5	0.56	0
6	GOL	B	1504	-	5,5,5	0.43	0	5,5,5	0.86	0
6	GOL	D	1504	-	5,5,5	0.53	0	5,5,5	0.83	0
6	GOL	B	1505	-	5,5,5	0.42	0	5,5,5	1.19	1 (20%)
6	GOL	D	1505	-	5,5,5	0.31	0	5,5,5	0.93	0
5	94K	D	1502	-	27,27,27	0.84	0	35,37,37	1.14	5 (14%)
8	DMS	B	1507	-	3,3,3	0.51	0	3,3,3	0.90	0
9	6EJ	C	101[B]	-	36,38,38	1.24	4 (11%)	46,55,55	1.72	11 (23%)
6	GOL	D	1506	-	5,5,5	0.51	0	5,5,5	0.79	0
6	GOL	A	101	-	5,5,5	0.43	0	5,5,5	0.71	0
6	GOL	D	1503	-	5,5,5	0.65	0	5,5,5	0.63	0
5	94K	B	1502	-	27,27,27	0.92	2 (7%)	35,37,37	1.34	6 (17%)

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
6	GOL	C	102	-	-	4/4/4/4	-
9	6EJ	C	101[A]	-	-	2/9/34/34	0/6/6/6
6	GOL	B	1503	-	-	4/4/4/4	-
6	GOL	B	1504	-	-	0/4/4/4	-
6	GOL	D	1504	-	-	2/4/4/4	-
6	GOL	B	1505	-	-	4/4/4/4	-
6	GOL	D	1505	-	-	4/4/4/4	-
5	94K	D	1502	-	-	2/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	6EJ	C	101[B]	-	-	2/9/34/34	0/6/6/6
6	GOL	D	1506	-	-	2/4/4/4	-
6	GOL	A	101	-	-	0/4/4/4	-
6	GOL	D	1503	-	-	4/4/4/4	-
5	94K	B	1502	-	-	1/18/18/18	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	101[A]	6EJ	C8-N10	-3.67	1.34	1.38
9	C	101[B]	6EJ	C8-N10	-3.48	1.34	1.38
9	C	101[A]	6EJ	N31-N32	2.89	1.41	1.34
9	C	101[B]	6EJ	N31-N32	2.65	1.40	1.34
5	B	1502	94K	C6-C7	-2.55	1.42	1.49

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	101[A]	6EJ	C24-C23-N32	-5.14	119.80	122.53
9	C	101[B]	6EJ	C34-N10-C8	-4.21	120.03	123.50
9	C	101[A]	6EJ	C23-N32-N31	4.04	121.79	119.77
9	C	101[B]	6EJ	C24-C23-N32	-3.69	120.57	122.53
5	B	1502	94K	C6-C7-N9	-3.59	111.57	116.25

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1502	94K	N9-C10-C11-N12
6	B	1503	GOL	O1-C1-C2-C3
6	B	1505	GOL	O1-C1-C2-C3
6	D	1503	GOL	C1-C2-C3-O3
6	D	1505	GOL	C1-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 14 short contacts:

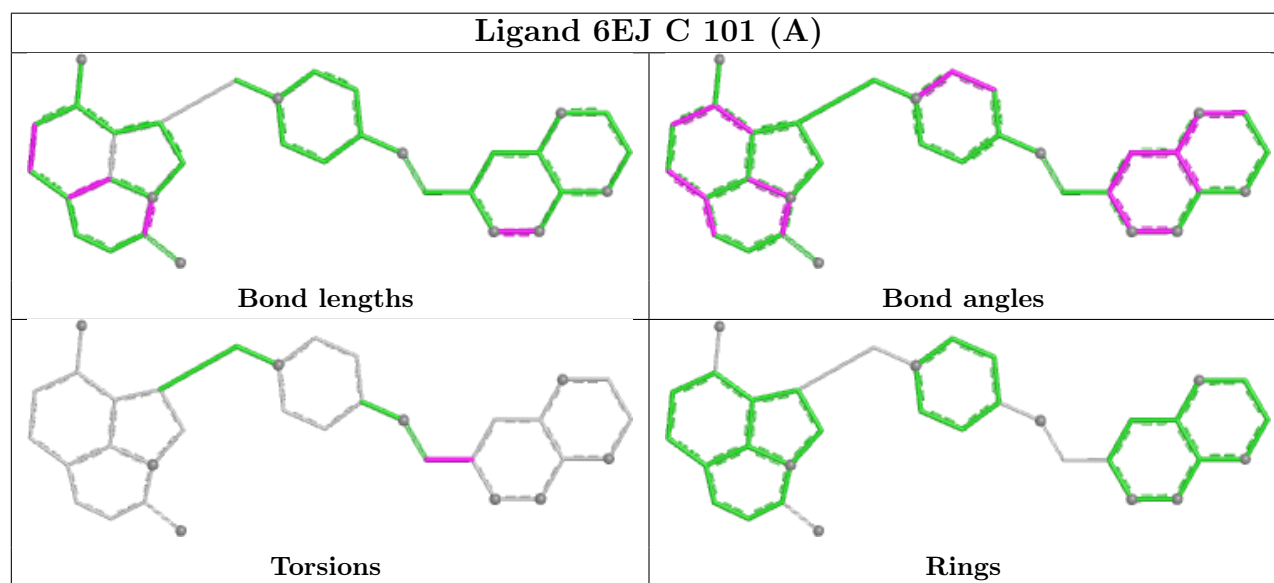
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	102	GOL	3	0
6	B	1503	GOL	1	0

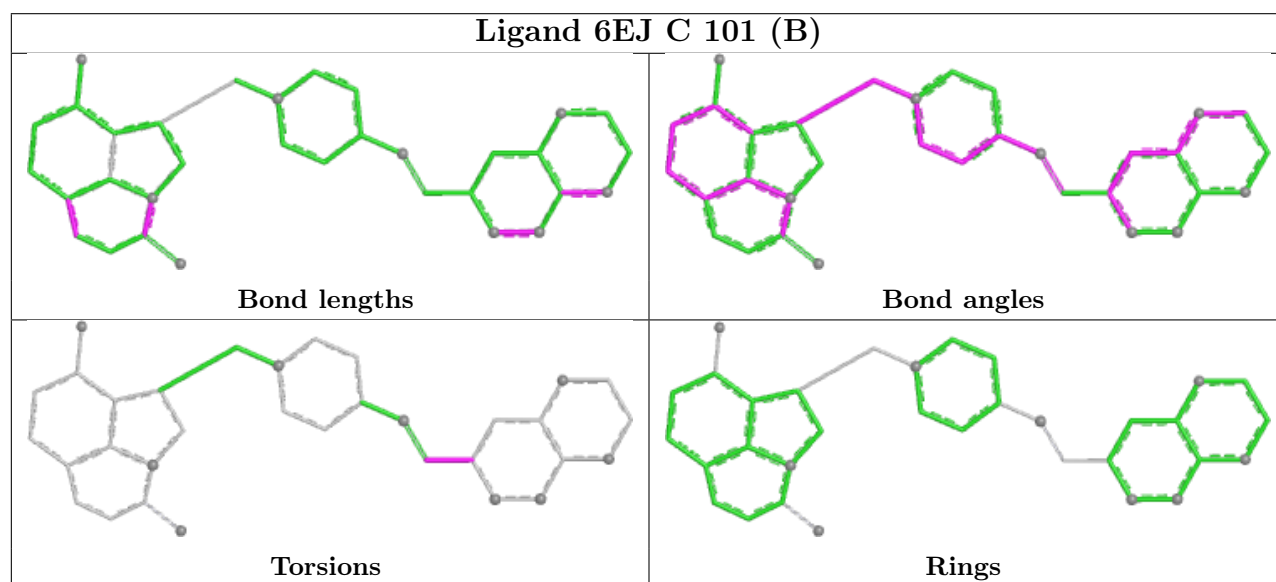
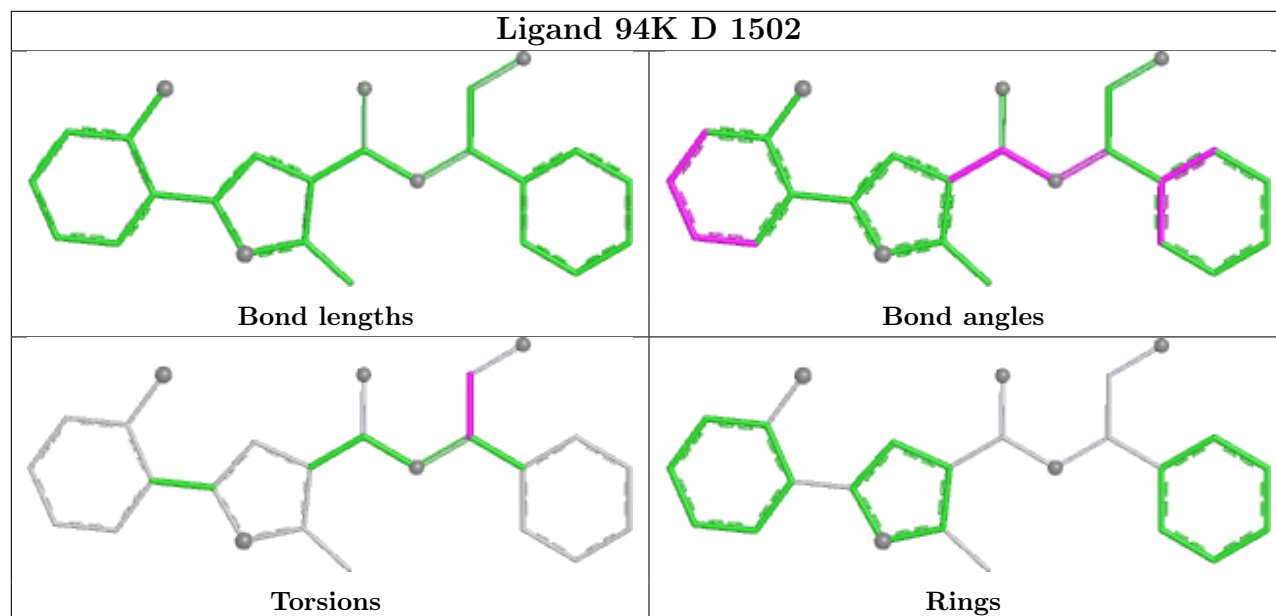
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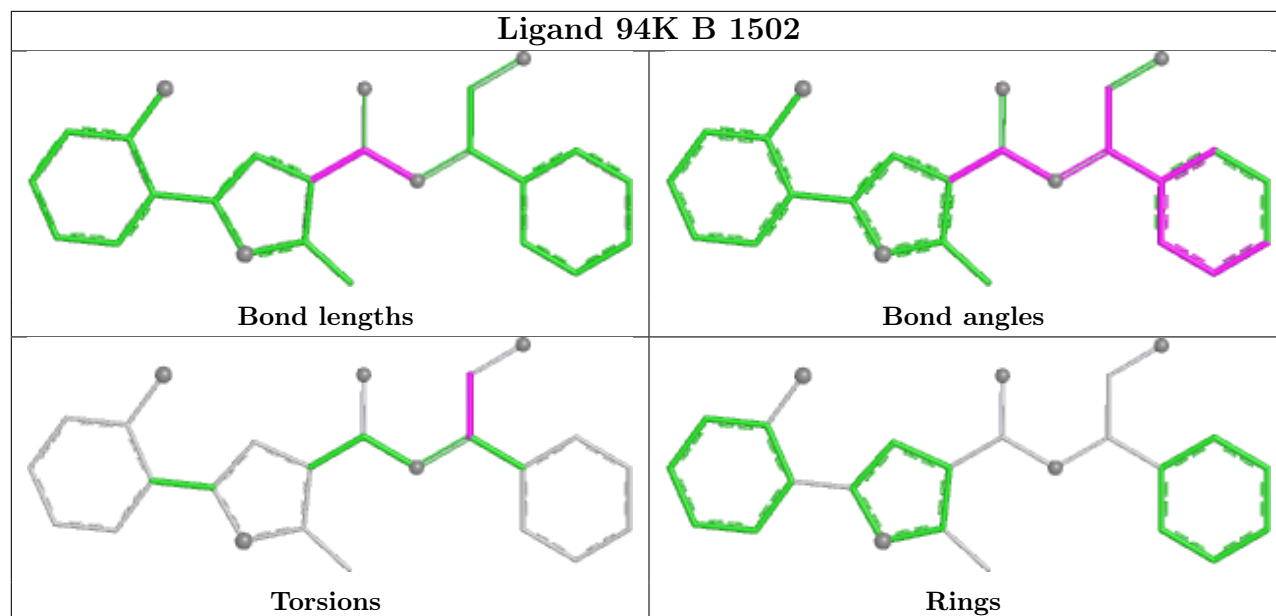
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1504	GOL	1	0
6	B	1505	GOL	1	0
5	D	1502	94K	1	0
8	B	1507	DMS	2	0
6	D	1506	GOL	1	0
6	A	101	GOL	3	0
5	B	1502	94K	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	672/692 (97%)	-0.52	6 (0%) 81 79	16, 38, 59, 88	28 (4%)
1	D	671/692 (96%)	-0.48	4 (0%) 85 84	15, 39, 69, 102	14 (2%)
2	E	8/8 (100%)	-1.12	0 100 100	29, 32, 44, 50	0
2	F	8/8 (100%)	-0.66	0 100 100	31, 36, 55, 66	1 (12%)
3	A	12/12 (100%)	-0.67	0 100 100	23, 33, 46, 70	4 (33%)
3	C	12/12 (100%)	-0.47	0 100 100	23, 31, 68, 69	3 (25%)
All	All	1383/1424 (97%)	-0.51	10 (0%) 84 83	15, 38, 64, 102	50 (3%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	581	LYS	3.6
1	B	581[A]	LYS	2.7
1	B	1439[A]	ASP	2.3
1	B	1436[A]	LEU	2.3
1	D	1056[A]	GLN	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

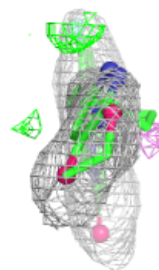
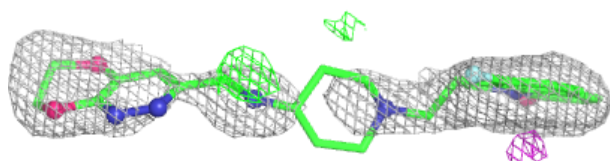
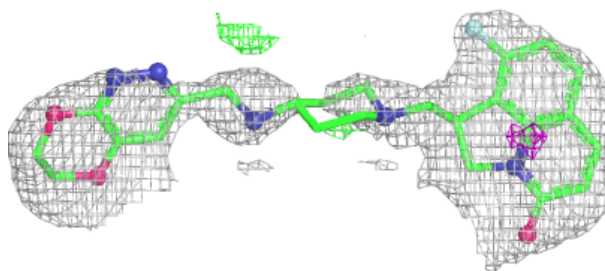
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	101	6/6	0.81	0.19	65,66,71,86	0
6	GOL	D	1506	6/6	0.82	0.16	54,65,73,78	0
6	GOL	D	1505	6/6	0.85	0.14	56,61,68,82	0
6	GOL	B	1503	6/6	0.88	0.12	52,58,62,65	0
6	GOL	C	102	6/6	0.88	0.13	45,57,66,68	0
8	DMS	B	1507	4/4	0.88	0.15	58,63,78,88	0
6	GOL	D	1504	6/6	0.90	0.13	59,62,70,71	0
6	GOL	B	1505	6/6	0.92	0.10	52,56,68,73	0
9	6EJ	C	101[A]	33/33	0.93	0.12	38,45,50,50	33
9	6EJ	C	101[B]	33/33	0.93	0.12	35,41,51,59	33
6	GOL	B	1504	6/6	0.95	0.08	38,51,58,58	0
6	GOL	D	1503	6/6	0.95	0.08	32,52,59,65	0
5	94K	D	1502	25/25	0.97	0.07	29,40,49,58	0
5	94K	B	1502	25/25	0.97	0.06	28,37,47,47	0
7	NA	B	1506	1/1	0.97	0.05	40,40,40,40	0
4	MN	D	1501	1/1	1.00	0.03	48,48,48,48	0
4	MN	B	1501	1/1	1.00	0.01	41,41,41,41	0

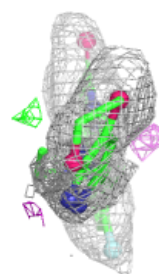
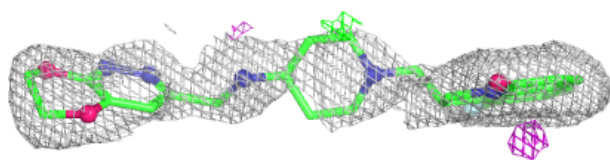
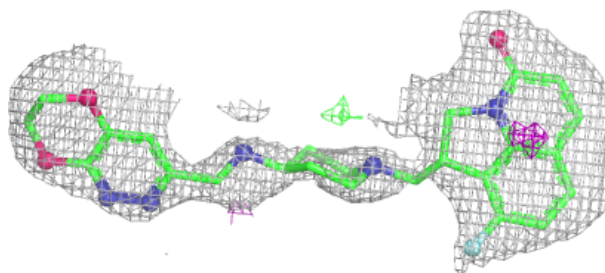
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6EJ C 101 (A):

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

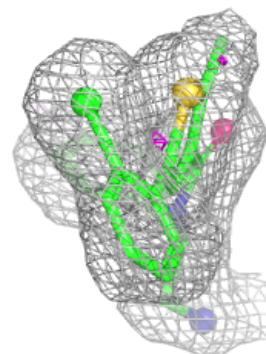
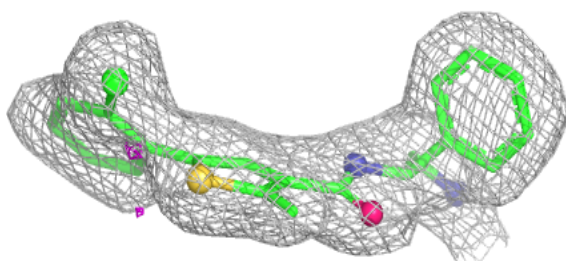
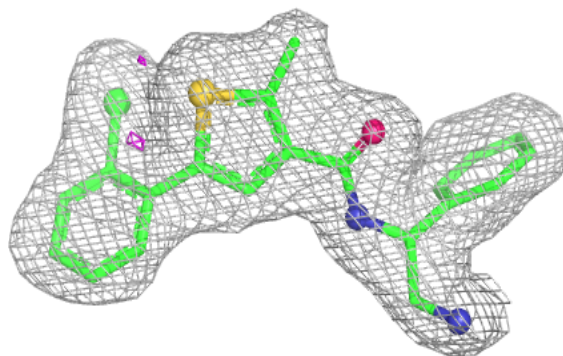
**Electron density around 6EJ C 101 (B):**

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

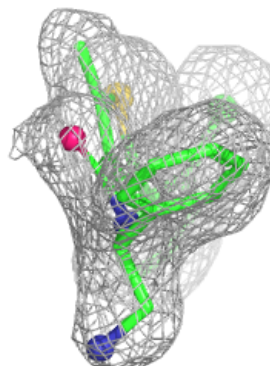
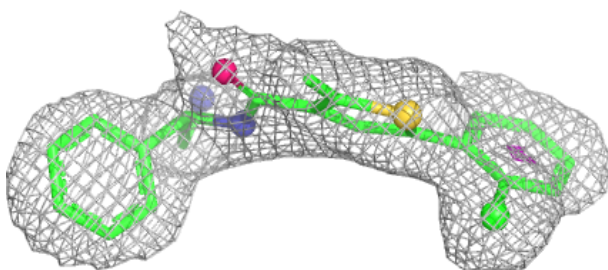
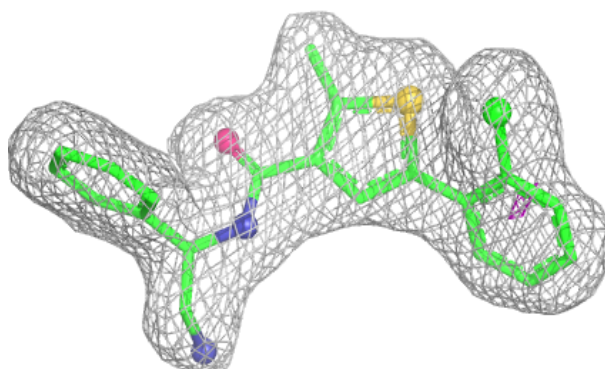


Electron density around 94K D 1502:

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

**Electron density around 94K 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.