



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 08:35 PM BST

PDB ID : 6FQM
Title : 3.06A COMPLEX OF S.AUREUS GYRASE with imidazopyrazinone T1 AND DNA
Authors : Bax, B.D.; Germe, T.; Basque, E.; Maxwell, A.
Deposited on : 2018-02-14
Resolution : 3.06 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 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

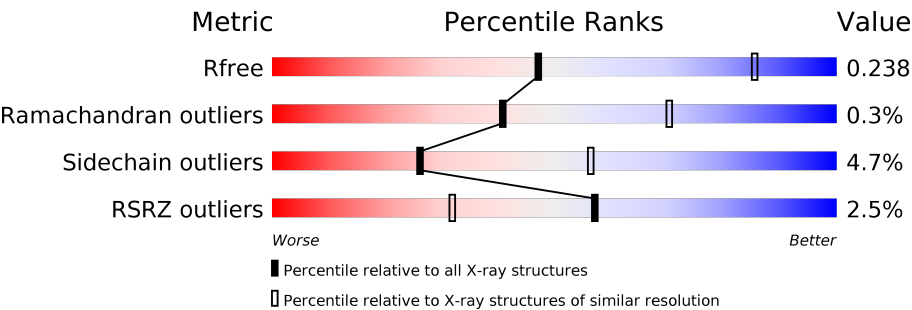
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	1754 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	B	201	
1	b	201	
1	d	201	
2	A	490	
2	C	490	
2	a	490	
2	c	490	

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Mol	Chain	Length	Quality of chain
3	D	202	<div><div></div><div>3%</div><div>70%</div><div>26%</div></div>
4	E	20	<div><div></div><div>95%</div><div>5%</div></div>
4	F	20	<div><div></div><div>85%</div><div>15%</div></div>
4	e	20	<div><div></div><div>90%</div><div>5%</div><div>5%</div></div>
4	f	20	<div><div></div><div>5%</div><div>95%</div><div>5%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21111 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	156	Total	C	N	O	S	0	1	0
			1176	751	191	225	9			
1	b	160	Total	C	N	O	S	0	0	0
			1196	760	198	231	7			
1	d	150	Total	C	N	O	S	0	0	0
			1097	692	185	213	7			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	THR	deletion	UNP P66937
B	?	-	GLN	deletion	UNP P66937
B	?	-	GLY	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	GLN	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	VAL	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	ASN	deletion	UNP P66937
B	?	-	ASP	deletion	UNP P66937
B	?	-	ARG	deletion	UNP P66937
B	?	-	GLU	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	ASP	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P66937
B	?	-	GLU	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	ASN	deletion	UNP P66937
B	?	-	PRO	deletion	UNP P66937
B	?	-	THR	deletion	UNP P66937
B	?	-	PRO	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	TRP	deletion	UNP P66937
B	?	-	SER	deletion	UNP P66937
B	?	-	ILE	deletion	UNP P66937
B	578	THR	ALA	conflict	UNP P66937
B	579	GLY	ARG	conflict	UNP P66937
b	?	-	LEU	deletion	UNP P66937
b	?	-	TYR	deletion	UNP P66937
b	?	-	LYS	deletion	UNP P66937
b	?	-	LEU	deletion	UNP P66937
b	?	-	THR	deletion	UNP P66937
b	?	-	GLN	deletion	UNP P66937
b	?	-	GLY	deletion	UNP P66937
b	?	-	LYS	deletion	UNP P66937
b	?	-	GLN	deletion	UNP P66937
b	?	-	LYS	deletion	UNP P66937
b	?	-	TYR	deletion	UNP P66937
b	?	-	TYR	deletion	UNP P66937
b	?	-	VAL	deletion	UNP P66937
b	?	-	TYR	deletion	UNP P66937
b	?	-	ASN	deletion	UNP P66937
b	?	-	ASP	deletion	UNP P66937
b	?	-	ARG	deletion	UNP P66937
b	?	-	GLU	deletion	UNP P66937
b	?	-	LEU	deletion	UNP P66937
b	?	-	ASP	deletion	UNP P66937
b	?	-	LYS	deletion	UNP P66937
b	?	-	LEU	deletion	UNP P66937
b	?	-	LYS	deletion	UNP P66937
b	?	-	SER	deletion	UNP P66937
b	?	-	GLU	deletion	UNP P66937
b	?	-	LEU	deletion	UNP P66937
b	?	-	ASN	deletion	UNP P66937
b	?	-	PRO	deletion	UNP P66937
b	?	-	THR	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
b	?	-	PRO	deletion	UNP P66937
b	?	-	LYS	deletion	UNP P66937
b	?	-	TRP	deletion	UNP P66937
b	?	-	SER	deletion	UNP P66937
b	?	-	ILE	deletion	UNP P66937
b	578	THR	ALA	conflict	UNP P66937
b	579	GLY	ARG	conflict	UNP P66937
d	?	-	LEU	deletion	UNP P66937
d	?	-	TYR	deletion	UNP P66937
d	?	-	LYS	deletion	UNP P66937
d	?	-	LEU	deletion	UNP P66937
d	?	-	THR	deletion	UNP P66937
d	?	-	GLN	deletion	UNP P66937
d	?	-	GLY	deletion	UNP P66937
d	?	-	LYS	deletion	UNP P66937
d	?	-	GLN	deletion	UNP P66937
d	?	-	LYS	deletion	UNP P66937
d	?	-	TYR	deletion	UNP P66937
d	?	-	TYR	deletion	UNP P66937
d	?	-	VAL	deletion	UNP P66937
d	?	-	TYR	deletion	UNP P66937
d	?	-	ASN	deletion	UNP P66937
d	?	-	ASP	deletion	UNP P66937
d	?	-	ARG	deletion	UNP P66937
d	?	-	GLU	deletion	UNP P66937
d	?	-	LEU	deletion	UNP P66937
d	?	-	ASP	deletion	UNP P66937
d	?	-	LYS	deletion	UNP P66937
d	?	-	LEU	deletion	UNP P66937
d	?	-	LYS	deletion	UNP P66937
d	?	-	SER	deletion	UNP P66937
d	?	-	GLU	deletion	UNP P66937
d	?	-	LEU	deletion	UNP P66937
d	?	-	ASN	deletion	UNP P66937
d	?	-	PRO	deletion	UNP P66937
d	?	-	THR	deletion	UNP P66937
d	?	-	PRO	deletion	UNP P66937
d	?	-	LYS	deletion	UNP P66937
d	?	-	TRP	deletion	UNP P66937
d	?	-	SER	deletion	UNP P66937
d	?	-	ILE	deletion	UNP P66937
d	578	THR	ALA	conflict	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
d	579	GLY	ARG	conflict	UNP P66937

- Molecule 2 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	482	Total	C	N	O	P	S	0	2	0
			3696	2303	664	712	1	16			
2	C	481	Total	C	N	O	P	S	0	2	0
			3696	2301	670	708	1	16			
2	a	474	Total	C	N	O	P	S	0	1	0
			3600	2243	641	699	1	16			
2	c	480	Total	C	N	O	P	S	0	2	0
			3687	2296	669	705	1	16			

- Molecule 3 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	150	Total	C	N	O	S	0	0	0
			1135	724	196	210	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	409	MET	-	initiating methionine	UNP P66937
D	578	THR	ALA	conflict	UNP P66937
D	579	GLY	ARG	conflict	UNP P66937

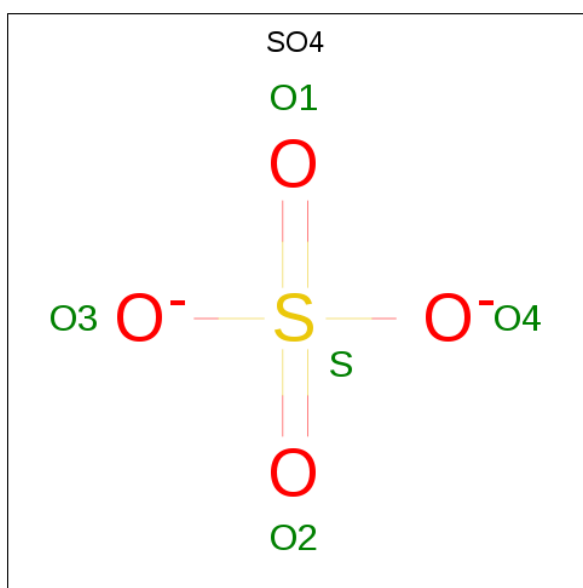
- Molecule 4 is a DNA chain called DNA (5'-D(*GP*AP*GP*AP*GP*TP*AP*T*GP*GP*C
P*CP*AP*TP*AP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	19	Total	C	N	O	P	0	0	0
			383	185	72	109	17			
4	F	20	Total	C	N	O	P	0	0	0
			403	195	74	116	18			
4	e	19	Total	C	N	O	P	0	0	0
			383	185	72	109	17			
4	f	20	Total	C	N	O	P	0	2	0
			416	201	74	121	20			

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

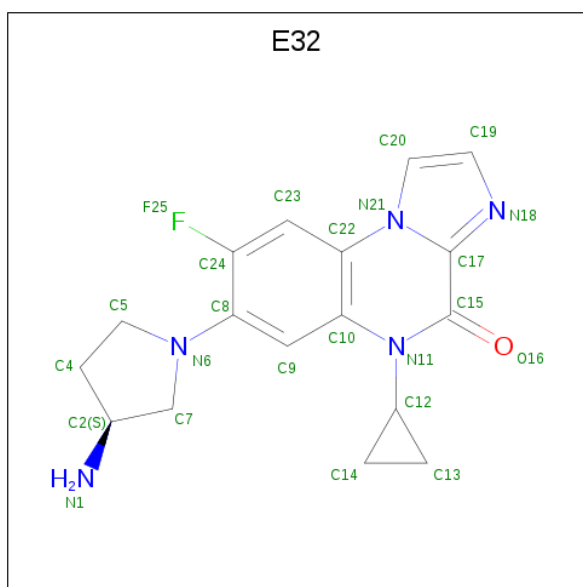
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	d	1	Total	Mn	0	0
			1	1		
5	B	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		
5	b	1	Total	Mn	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



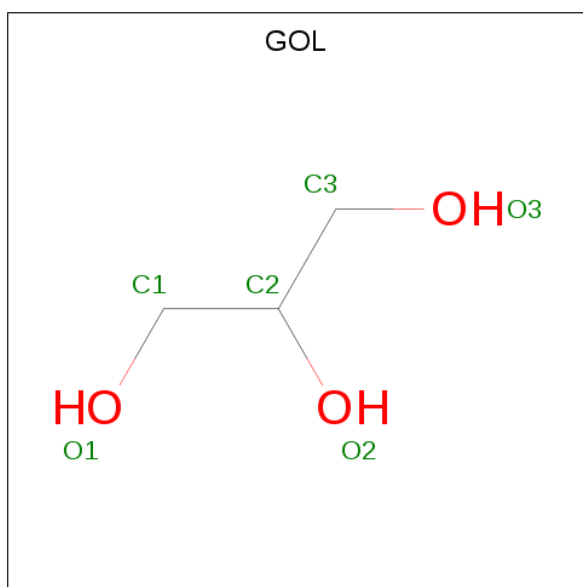
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	c	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 7-[(3 {S})-3-azanylpyrrolidin-1-yl]-5-cyclopropyl-8-fluoranyl-imidazo[1,2-a]quinoxalin-4-one (three-letter code: E32) (formula: C₁₇H₁₈FN₅O) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	E	1	Total	C	F	N	O	0	0
			24	17	1	5	1		
7	E	1	Total	C	F	N	O	0	0
			24	17	1	5	1		
7	F	1	Total	C	F	N	O	0	0
			24	17	1	5	1		
7	e	1	Total	C	F	N	O	0	0
			24	17	1	5	1		
7	f	1	Total	C	F	N	O	0	0
			24	17	1	5	1		
7	f	1	Total	C	F	N	O	0	1
			48	34	2	10	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	5	Total	O	0	0
			5	5		
9	A	3	Total	O	0	0
			3	3		
9	D	5	Total	O	0	0
			5	5		
9	C	13	Total	O	0	0
			13	13		
9	E	3	Total	O	0	0
			3	3		
9	F	1	Total	O	0	0
			1	1		
9	b	5	Total	O	0	0
			5	5		
9	a	6	Total	O	0	0
			6	6		
9	d	4	Total	O	0	0
			4	4		
9	c	5	Total	O	0	0
			5	5		
9	e	2	Total	O	0	0
			2	2		

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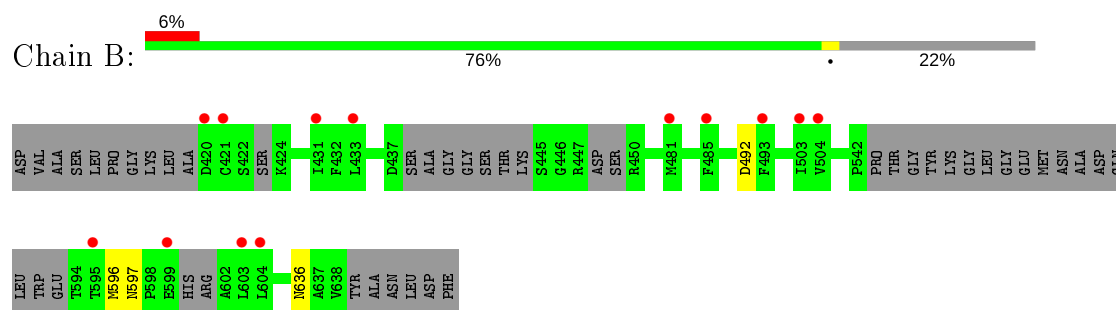
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	f	3	Total	O	0	0
			3	3		

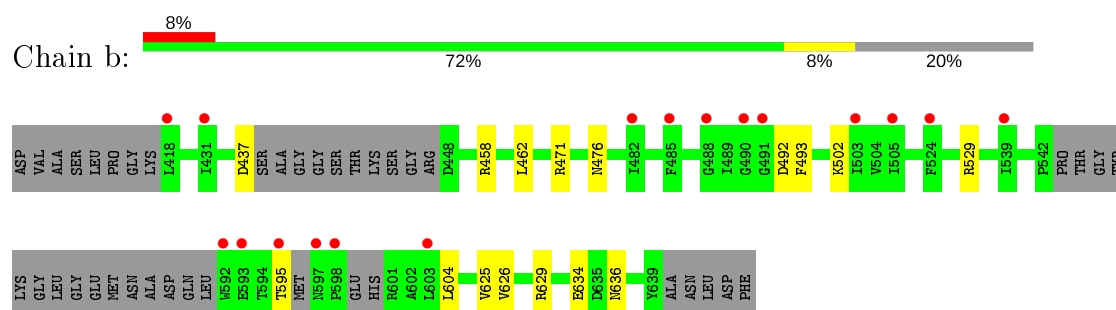
3 Residue-property plots [i](#)

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.

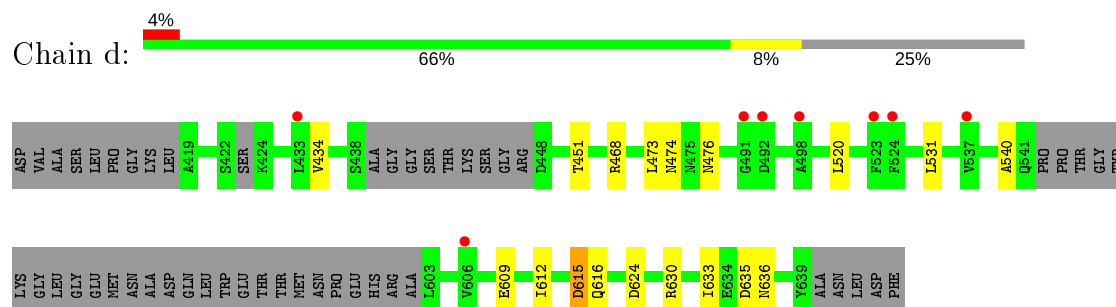
• Molecule 1: DNA gyrase subunit B



• Molecule 1: DNA gyrase subunit B

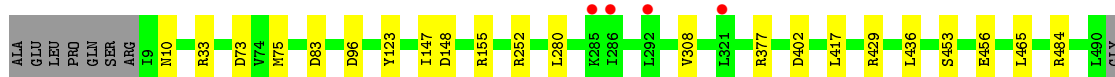


• Molecule 1: DNA gyrase subunit B



• Molecule 2: DNA gyrase subunit A





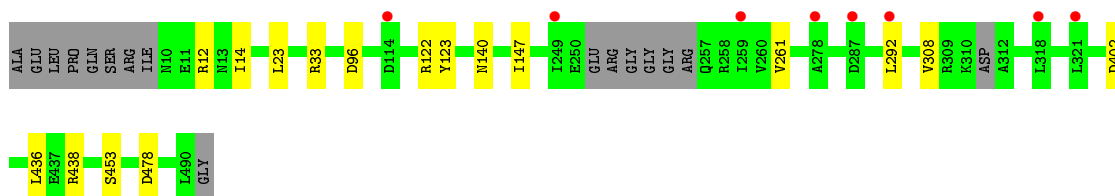
- Molecule 2: DNA gyrase subunit A

Chain C: 93% 5%



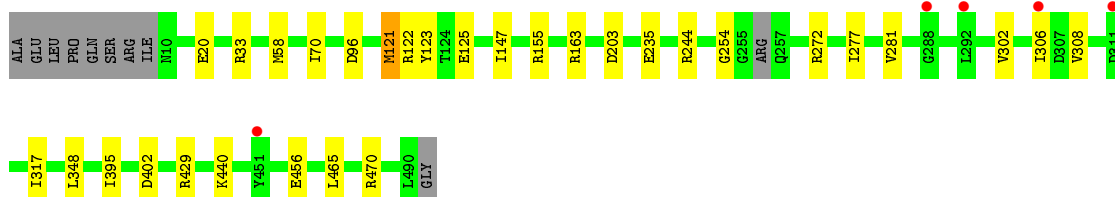
- Molecule 2: DNA gyrase subunit A

Chain a: 93% 2%



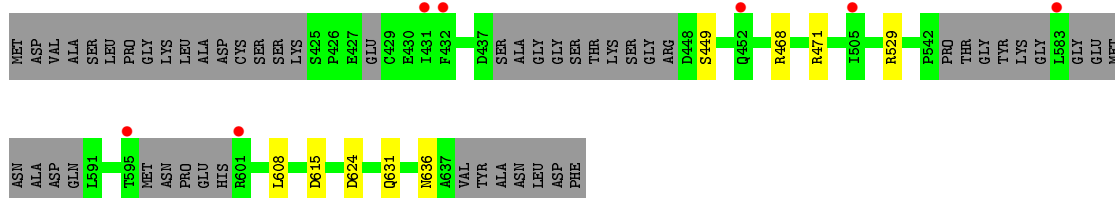
- Molecule 2: DNA gyrase subunit A

Chain c: 92% 6%



- Molecule 3: DNA gyrase subunit B

Chain D: 70% 3% 26%

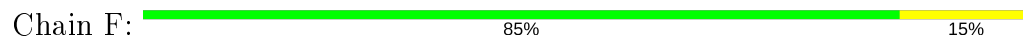


- Molecule 4: DNA (5'-D(*GP*AP*GP*AP*GP*TP*AP*T*GP*GP*CP*CP*AP*TP*AP*CP*TP*CP*T)-3')

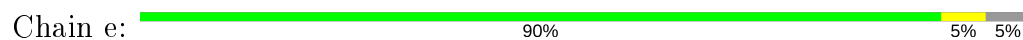
Chain E: 95% 5%



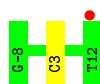
- Molecule 4: DNA (5'-D(*GP*AP*GP*AP*GP*TP*AP*T*GP*GP*CP*CP*AP*TP*AP*CP*TP*CP*T)-3')



- Molecule 4: DNA (5'-D(*GP*AP*GP*AP*GP*TP*AP*T*GP*GP*CP*CP*AP*TP*AP*CP*TP*CP*T)-3')



- Molecule 4: DNA (5'-D(*GP*AP*GP*AP*GP*TP*AP*T*GP*GP*CP*CP*AP*TP*AP*CP*TP*CP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.34Å 171.71Å 124.87Å 90.00° 102.86° 90.00°	Depositor
Resolution (Å)	59.90 – 3.06 59.90 – 3.06	Depositor EDS
% Data completeness (in resolution range)	98.6 (59.90-3.06) 98.6 (59.90-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.195 , 0.234 0.197 , 0.238	Depositor DCC
R_{free} test set	3323 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 83.3	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	0.95	EDS
Total number of atoms	21111	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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: GOL, PTR, MN, E32, SO4

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	0.70	0/1189	0.94	0/1608
1	b	0.69	0/1210	0.93	2/1641 (0.1%)
1	d	0.71	0/1108	0.99	6/1501 (0.4%)
2	A	0.66	0/3726	0.88	6/5047 (0.1%)
2	C	0.69	0/3726	0.89	9/5042 (0.2%)
2	a	0.65	0/3628	0.82	3/4917 (0.1%)
2	c	0.71	0/3716	0.94	9/5026 (0.2%)
3	D	0.69	0/1147	0.90	3/1549 (0.2%)
4	E	0.77	0/429	1.00	0/659
4	F	0.79	1/451 (0.2%)	1.04	2/693 (0.3%)
4	e	0.86	1/429 (0.2%)	0.93	0/659
4	f	0.72	0/463	0.99	1/708 (0.1%)
All	All	0.69	2/21222 (0.0%)	0.91	41/29050 (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
2	A	0	1
2	C	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	7	DA	O3'-P	-5.19	1.54	1.61
4	e	7	DA	O3'-P	-5.04	1.55	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	75	MET	CG-SD-CE	-9.17	85.53	100.20
2	C	47	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	d	468	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	b	629	ARG	NE-CZ-NH2	-7.29	116.65	120.30
2	C	465	LEU	CB-CG-CD2	-7.26	98.66	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	484	ARG	Mainchain
2	C	163	ARG	Mainchain
2	C	97	PHE	Mainchain

5.2 Too-close contacts ⓘ

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

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	B	145/201 (72%)	141 (97%)	4 (3%)	0	100	100
1	b	150/201 (75%)	147 (98%)	2 (1%)	1 (1%)	22	52
1	d	142/201 (71%)	137 (96%)	4 (3%)	1 (1%)	22	52
2	A	481/490 (98%)	465 (97%)	15 (3%)	1 (0%)	47	77
2	C	480/490 (98%)	464 (97%)	15 (3%)	1 (0%)	47	77
2	a	468/490 (96%)	452 (97%)	15 (3%)	1 (0%)	47	77
2	c	477/490 (97%)	459 (96%)	16 (3%)	2 (0%)	34	64
3	D	139/202 (69%)	137 (99%)	2 (1%)	0	100	100
All	All	2482/2765 (90%)	2402 (97%)	73 (3%)	7 (0%)	41	70

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	d	540	ALA
1	b	458	ARG
2	A	33	ARG
2	c	254	GLY
2	C	33	ARG

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	B	116/167 (70%)	112 (97%)	4 (3%)	37	67
1	b	118/167 (71%)	106 (90%)	12 (10%)	7	24
1	d	104/167 (62%)	91 (88%)	13 (12%)	4	16
2	A	381/422 (90%)	367 (96%)	14 (4%)	34	64
2	C	380/422 (90%)	366 (96%)	14 (4%)	34	64
2	a	366/422 (87%)	354 (97%)	12 (3%)	38	67
2	c	377/422 (89%)	357 (95%)	20 (5%)	22	51
3	D	109/168 (65%)	103 (94%)	6 (6%)	21	50
All	All	1951/2357 (83%)	1856 (95%)	95 (5%)	26	55

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	492	ASP
2	a	122	ARG
2	c	308	VAL
1	b	502	LYS
1	b	625	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	347	ASN
2	C	450	ASN
2	a	370	ASN
2	C	201	ASN
1	d	476	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
2	PTR	C	123	2,4	15,16,17	1.22	1 (6%)	19,22,24	1.38	2 (10%)
2	PTR	c	123	2,4	15,16,17	1.10	1 (6%)	19,22,24	1.76	4 (21%)
2	PTR	A	123	2,4	15,16,17	0.85	0	19,22,24	1.52	3 (15%)
2	PTR	a	123	2,4	15,16,17	0.86	0	19,22,24	1.16	1 (5%)

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
2	PTR	C	123	2,4	-	2/10/11/13	0/1/1/1
2	PTR	c	123	2,4	-	2/10/11/13	0/1/1/1
2	PTR	A	123	2,4	-	2/10/11/13	0/1/1/1
2	PTR	a	123	2,4	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	123	PTR	CE1-CD1	2.65	1.43	1.38
2	c	123	PTR	P-O3P	-2.14	1.46	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	123	PTR	O3P-P-OH	-3.57	94.07	105.24
2	c	123	PTR	CB-CG-CD2	-3.33	114.30	120.91
2	C	123	PTR	O2P-P-O1P	3.28	123.51	110.68
2	c	123	PTR	O3P-P-O2P	2.93	118.84	107.64
2	c	123	PTR	O3P-P-OH	-2.85	96.34	105.24

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	c	123	PTR	O-C-CA-CB
2	C	123	PTR	CA-CB-CG-CD2
2	C	123	PTR	CA-CB-CG-CD1
2	A	123	PTR	CA-CB-CG-CD1
2	A	123	PTR	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
8	GOL	E	1002	-	5,5,5	0.64	0	5,5,5	0.37	0
7	E32	f	1002[B]	-	23,28,28	1.20	3 (13%)	15,43,43	1.66	3 (20%)
7	E32	f	1001	-	23,28,28	1.25	5 (21%)	15,43,43	2.95	5 (33%)
6	SO4	C	1101	-	4,4,4	0.36	0	6,6,6	0.25	0
6	SO4	c	1101	-	4,4,4	0.37	0	6,6,6	0.22	0
7	E32	F	101	-	23,28,28	1.29	3 (13%)	15,43,43	2.07	6 (40%)
7	E32	f	1002[A]	-	23,28,28	1.21	2 (8%)	15,43,43	1.48	3 (20%)
7	E32	E	1003	-	23,28,28	1.11	4 (17%)	15,43,43	2.61	8 (53%)
7	E32	e	1001	-	23,28,28	1.15	3 (13%)	15,43,43	1.75	6 (40%)
7	E32	E	1001	-	23,28,28	1.10	3 (13%)	15,43,43	1.76	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	E	1002	-	-	4/4/4/4	-
7	E32	f	1002[B]	-	-	3/8/19/19	0/5/5/5
7	E32	f	1001	-	-	3/8/19/19	0/5/5/5
7	E32	F	101	-	-	2/8/19/19	0/5/5/5
7	E32	f	1002[A]	-	-	2/8/19/19	0/5/5/5
7	E32	E	1003	-	-	4/8/19/19	0/5/5/5
7	E32	e	1001	-	-	4/8/19/19	0/5/5/5
7	E32	E	1001	-	-	4/8/19/19	0/5/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	f	1002[A]	E32	C17-N18	3.46	1.36	1.33
7	F	101	E32	C10-N11	2.90	1.42	1.39
7	e	1001	E32	C23-C24	2.75	1.39	1.35
7	f	1002[A]	E32	C23-C24	2.72	1.39	1.35
7	f	1002[B]	E32	C15-N11	2.66	1.42	1.38

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	1001	E32	F25-C24-C8	8.39	126.05	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	f	1001	E32	F25-C24-C23	-4.78	114.15	120.47
7	f	1002[B]	E32	F25-C24-C8	4.32	122.35	118.42
7	E	1003	E32	C4-C5-N6	-4.24	98.38	103.35
7	E	1003	E32	F25-C24-C8	4.19	122.23	118.42

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

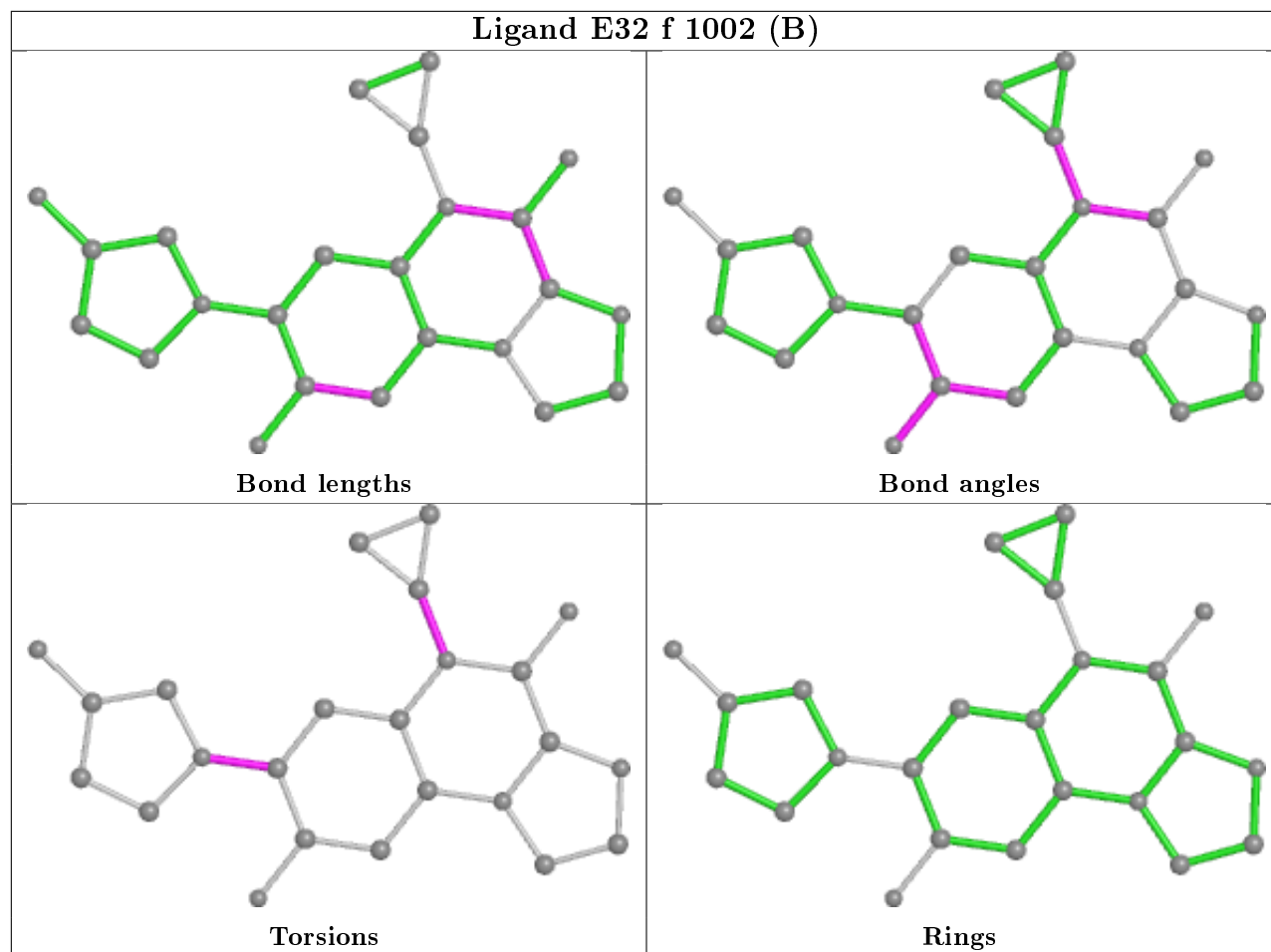
Mol	Chain	Res	Type	Atoms
7	f	1002[B]	E32	C14-C12-N11-C10
7	f	1002[B]	E32	C13-C12-N11-C10
7	f	1001	E32	C14-C12-N11-C10
7	f	1001	E32	C13-C12-N11-C10
7	f	1001	E32	C14-C12-N11-C15

There are no ring outliers.

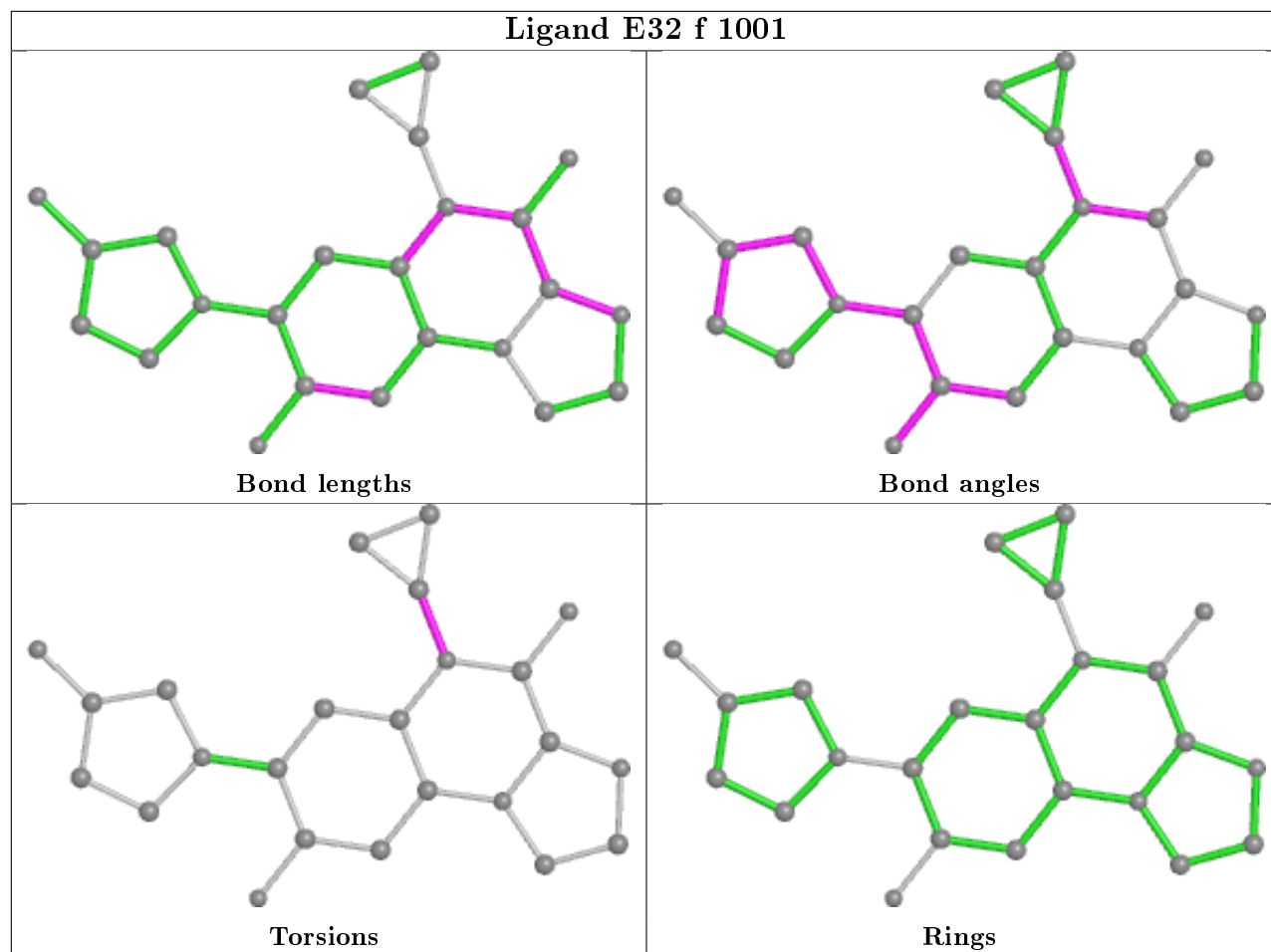
No monomer is involved in short contacts.

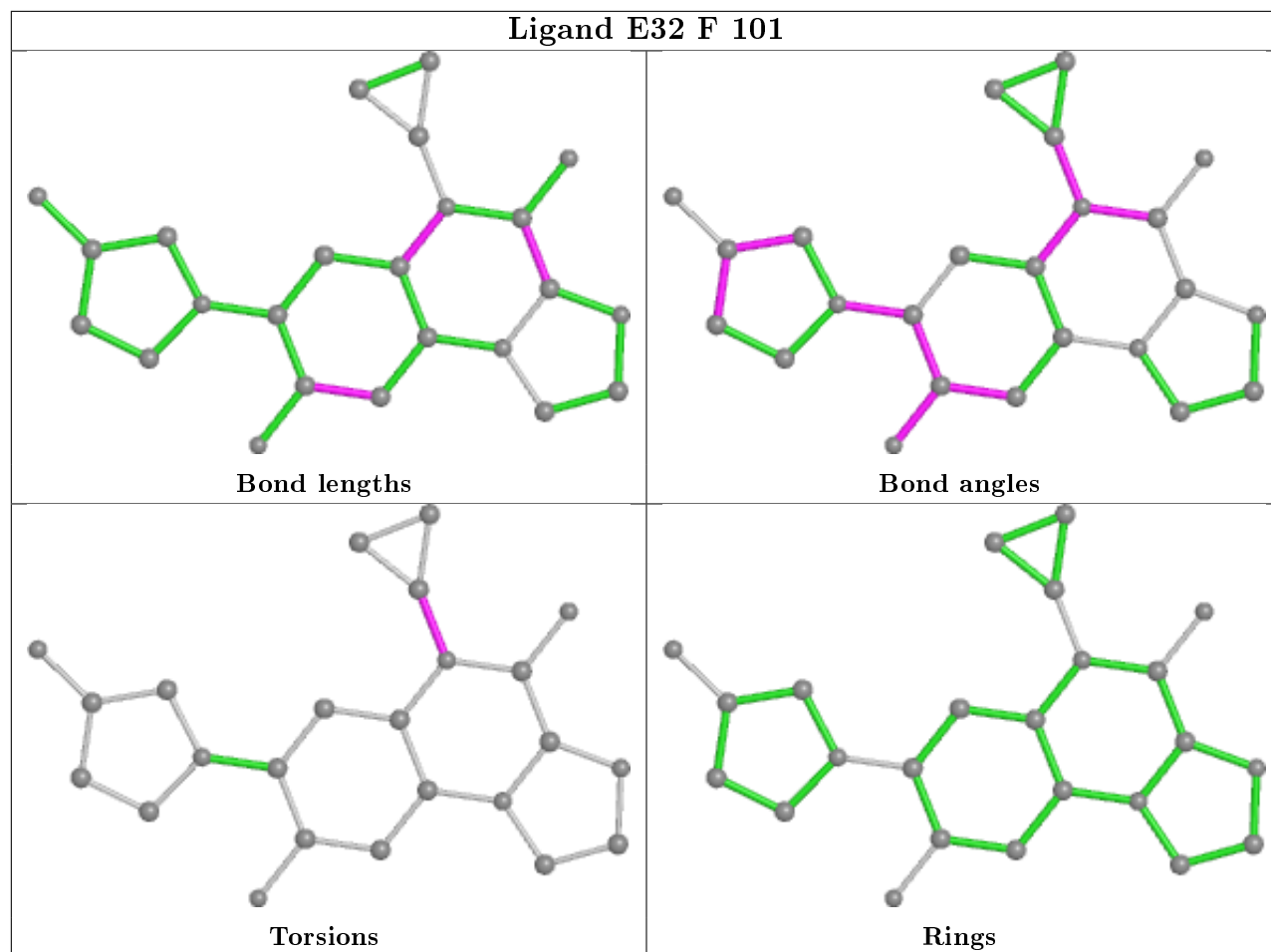
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

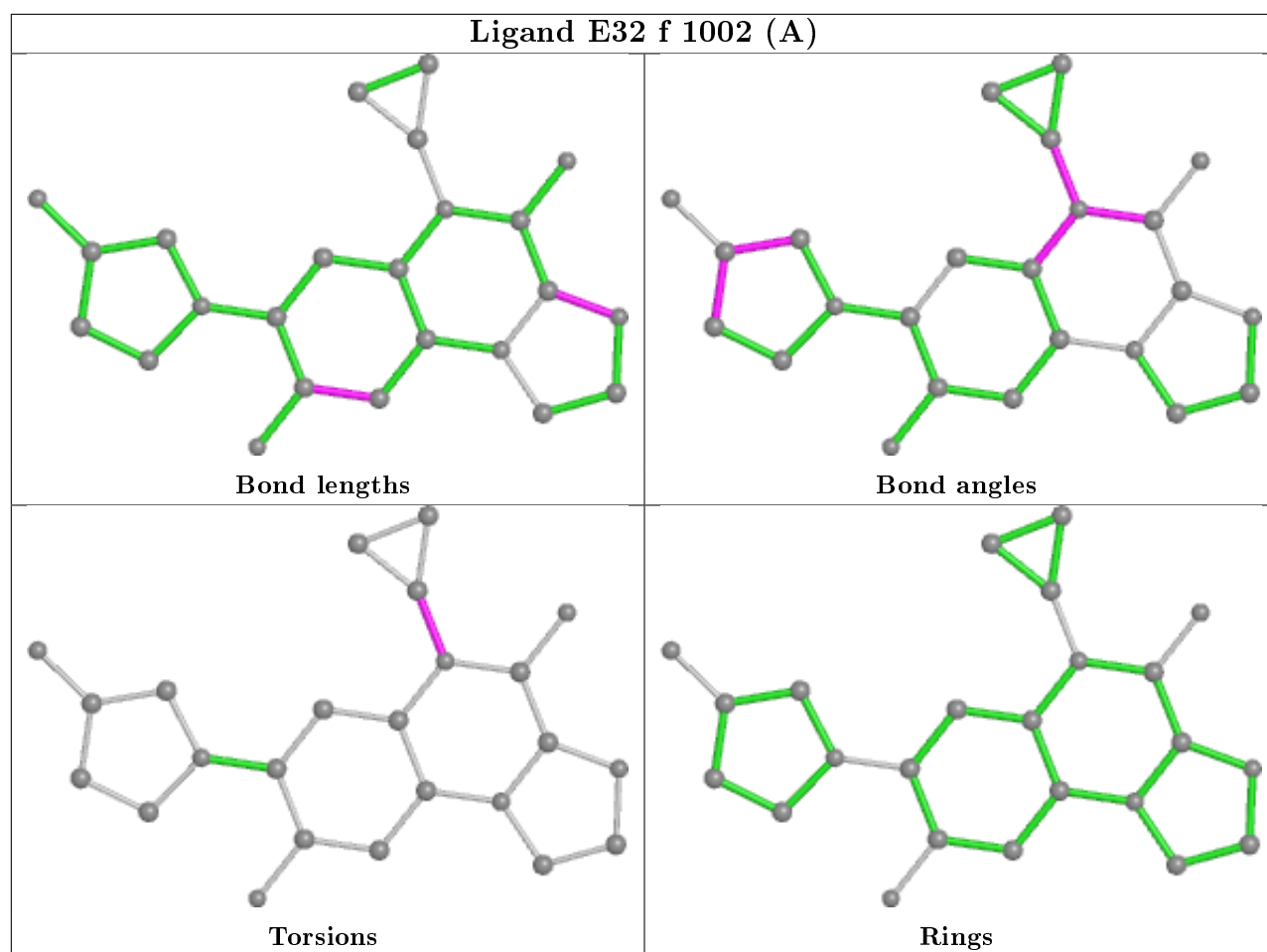
Ligand E32 f 1002 (B)

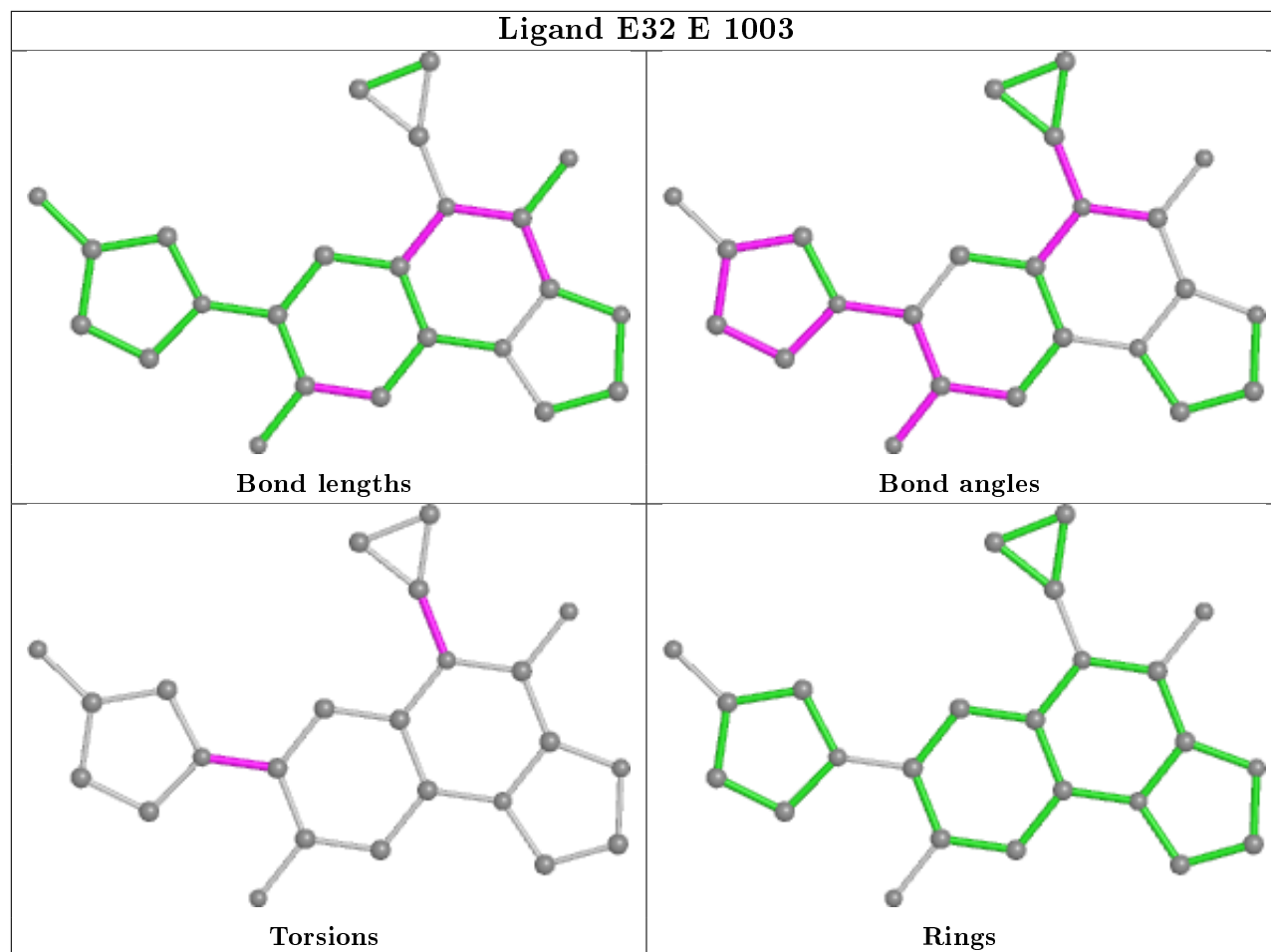


Ligand E32 f 1001

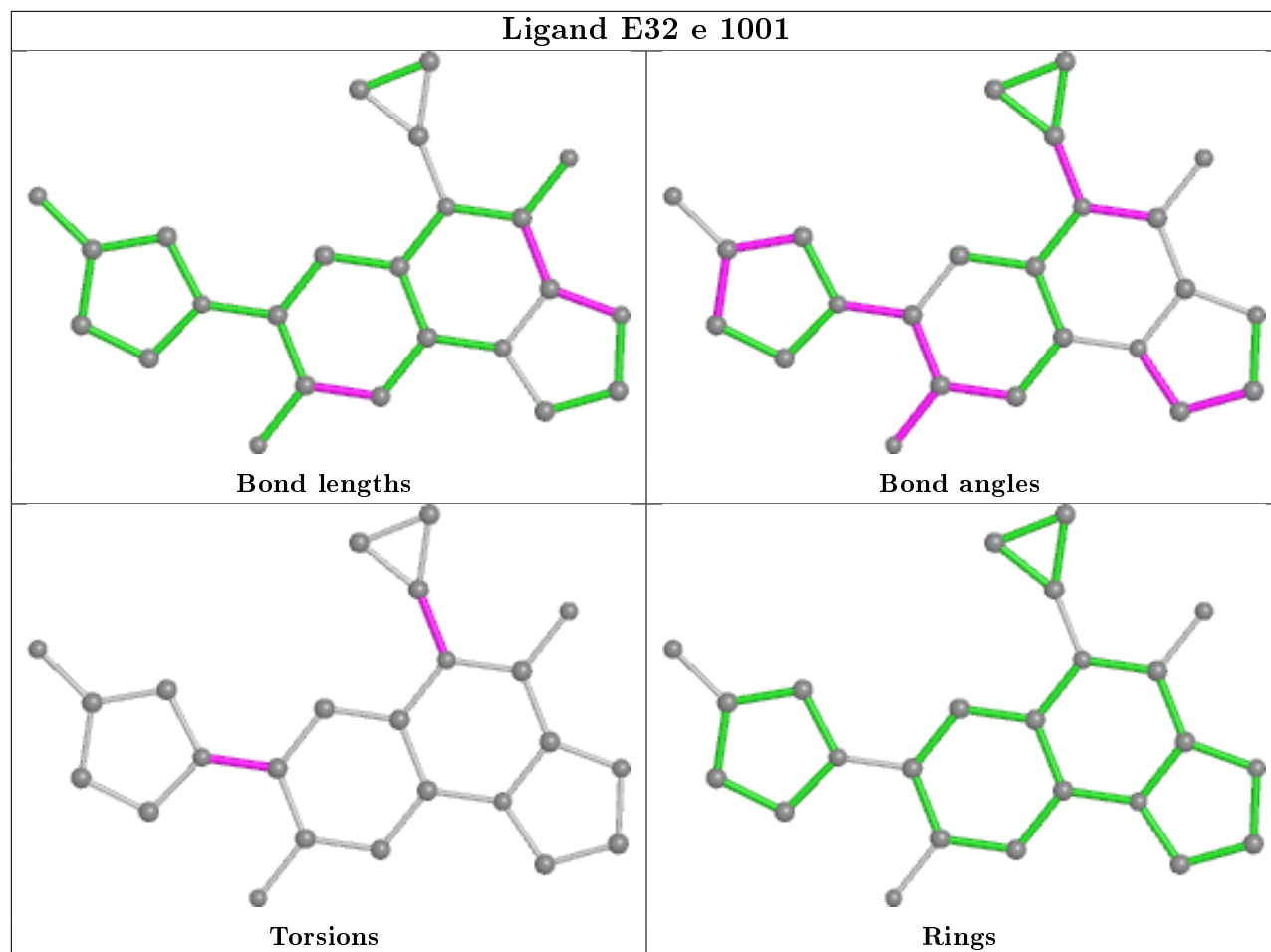


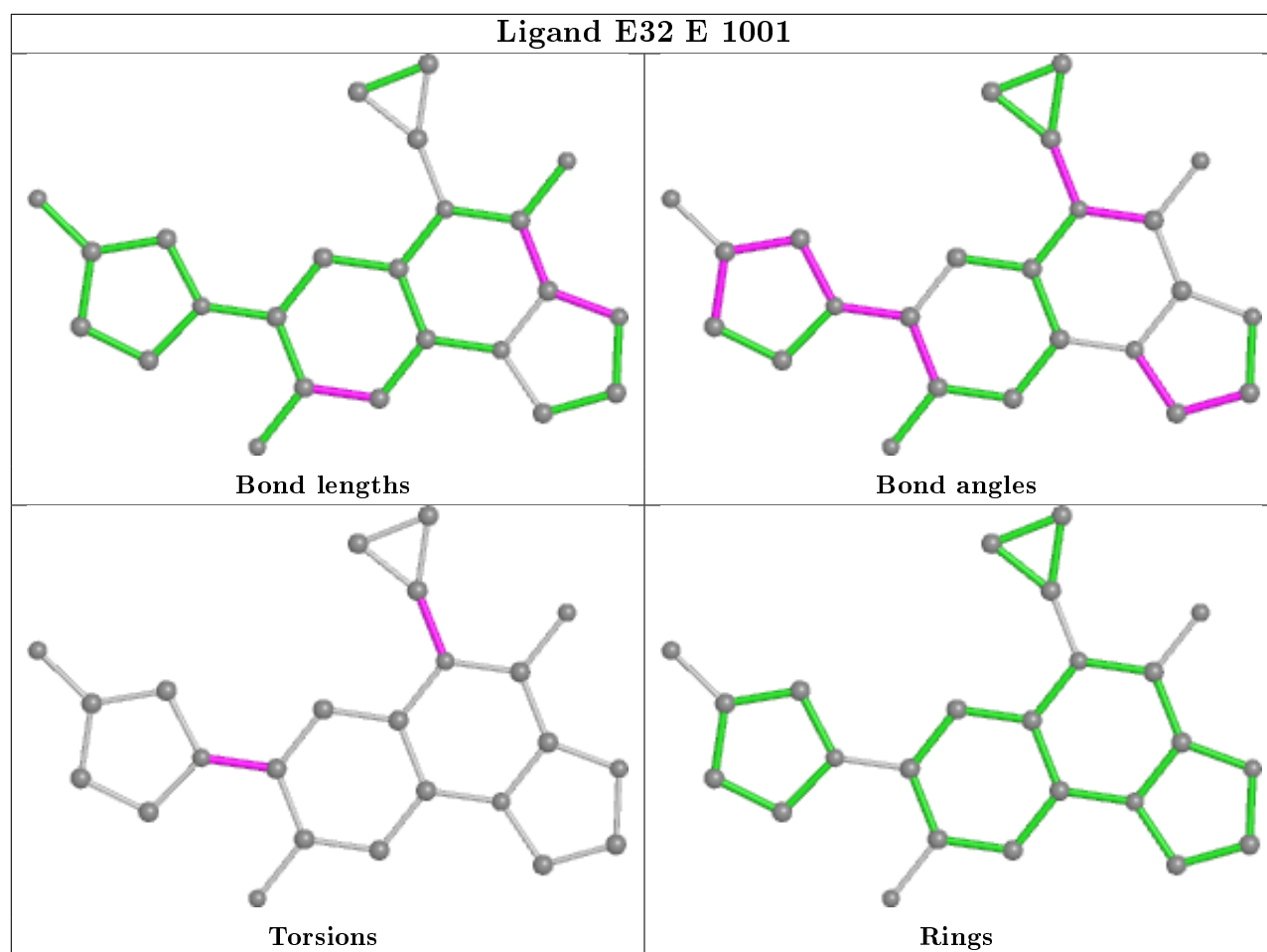






Ligand E32 e 1001





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	156/201 (77%)	0.24	13 (8%) 11 4	67, 113, 186, 214	0
1	b	160/201 (79%)	0.35	17 (10%) 6 2	73, 116, 194, 226	0
1	d	150/201 (74%)	0.23	8 (5%) 26 11	86, 129, 172, 193	0
2	A	481/490 (98%)	-0.22	4 (0%) 86 70	65, 98, 145, 170	0
2	C	480/490 (97%)	-0.29	1 (0%) 95 89	55, 86, 114, 141	0
2	a	473/490 (96%)	-0.14	8 (1%) 70 46	61, 96, 155, 204	0
2	c	479/490 (97%)	-0.18	5 (1%) 82 63	66, 97, 147, 179	0
3	D	150/202 (74%)	0.15	7 (4%) 31 14	70, 117, 176, 209	0
4	E	19/20 (95%)	-0.12	0 100 100	64, 75, 97, 109	0
4	F	20/20 (100%)	-0.08	0 100 100	65, 80, 117, 156	0
4	e	19/20 (95%)	-0.23	0 100 100	71, 82, 102, 103	0
4	f	20/20 (100%)	0.00	1 (5%) 28 12	65, 84, 122, 126	0
All	All	2607/2845 (91%)	-0.10	64 (2%) 57 32	55, 98, 157, 226	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	b	595	THR	7.0
1	B	599	GLU	5.2
1	b	418	LEU	5.0
4	f	12[A]	DT	4.3
2	a	287	ASP	3.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PTR	a	123	16/17	0.90	0.18	120,137,157,163	0
2	PTR	c	123	16/17	0.93	0.18	85,115,124,131	0
2	PTR	A	123	16/17	0.95	0.23	82,89,113,124	0
2	PTR	C	123	16/17	0.95	0.20	79,89,95,113	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

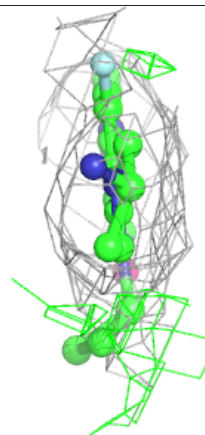
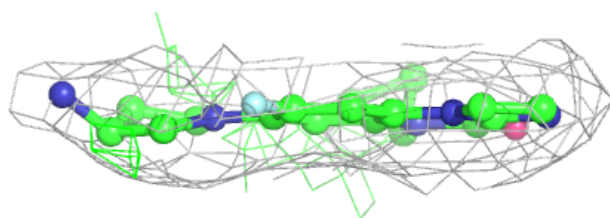
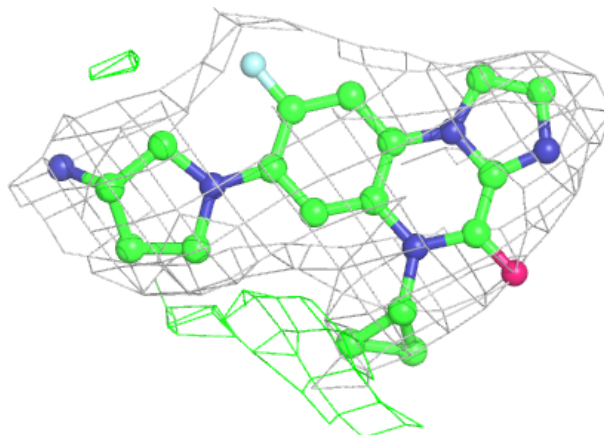
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	c	1101	5/5	0.86	0.23	132,136,148,148	0
7	E32	F	101	24/24	0.90	0.17	84,93,115,116	0
8	GOL	E	1002	6/6	0.92	0.21	74,86,91,92	0
7	E32	f	1002[A]	24/24	0.92	0.22	29,30,32,32	24
7	E32	f	1002[B]	24/24	0.92	0.22	93,126,150,154	24
5	MN	b	901	1/1	0.92	0.09	116,116,116,116	0
6	SO4	C	1101	5/5	0.93	0.17	131,138,143,153	0
5	MN	D	901	1/1	0.93	0.10	106,106,106,106	0
7	E32	f	1001	24/24	0.94	0.16	61,70,89,102	0
7	E32	e	1001	24/24	0.96	0.14	68,75,105,111	0
7	E32	E	1001	24/24	0.97	0.19	51,64,87,100	0
7	E32	E	1003	24/24	0.97	0.18	57,61,90,117	0
5	MN	d	901	1/1	0.98	0.04	129,129,129,129	0
5	MN	B	901	1/1	0.98	0.09	109,109,109,109	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.

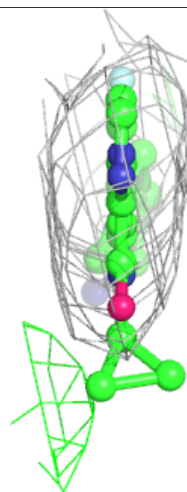
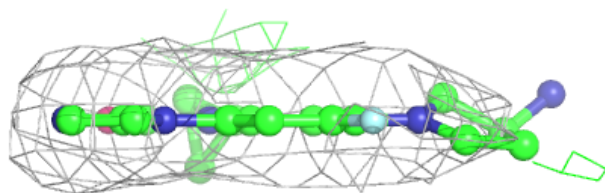
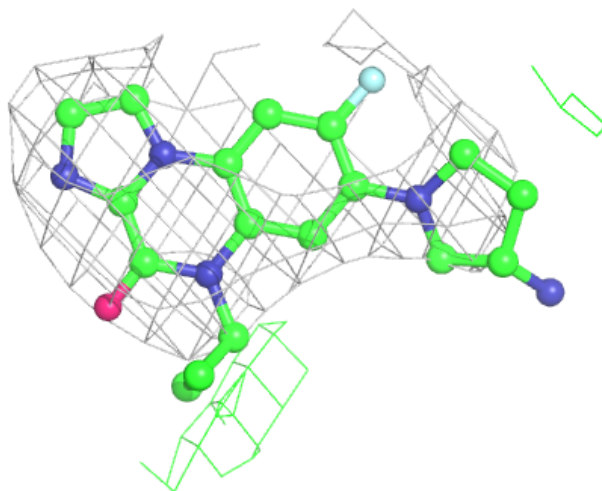
Electron density around E32 F 101:

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



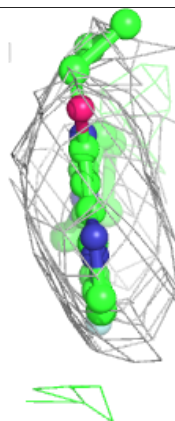
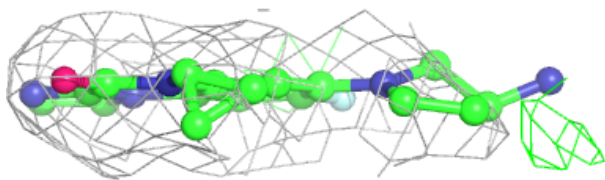
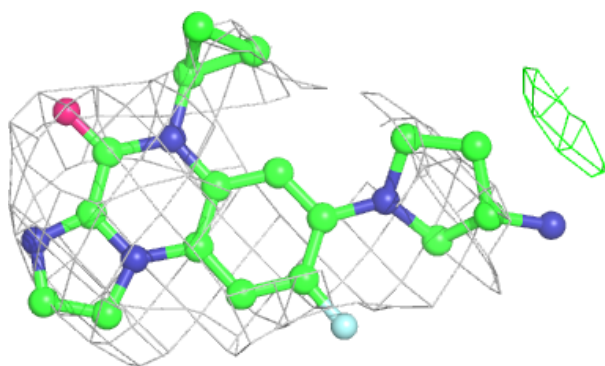
Electron density around E32 f 1002 (A):

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



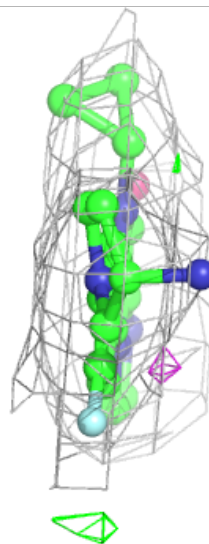
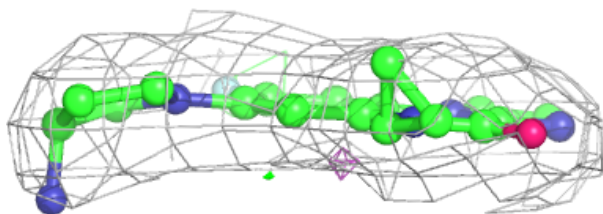
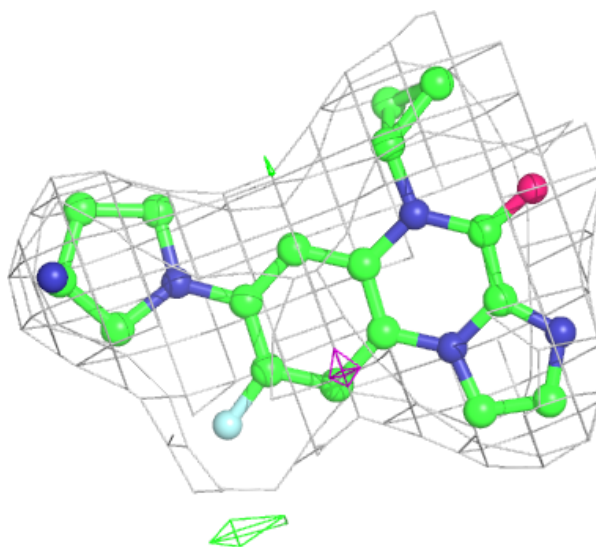
Electron density around E32 f 1002 (B):

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



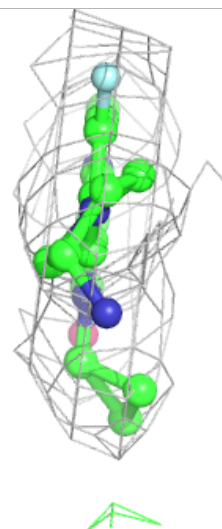
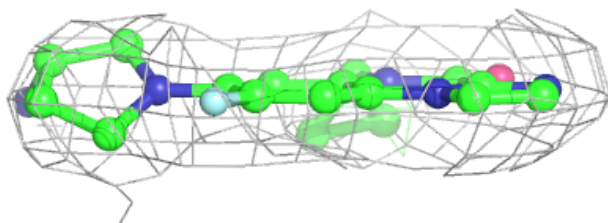
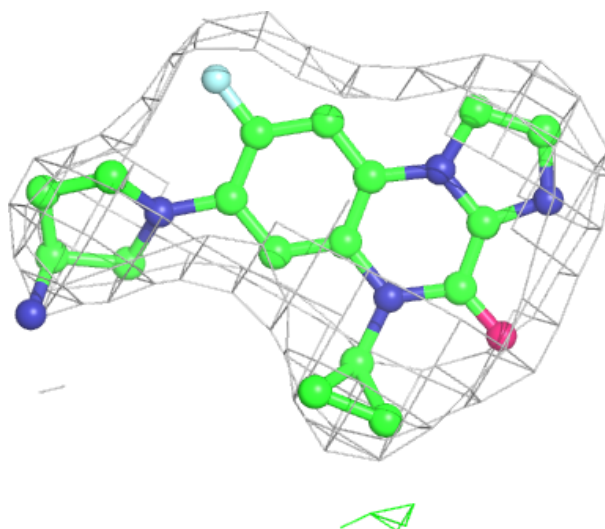
Electron density around E32 f 1001:

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



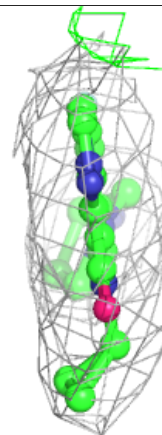
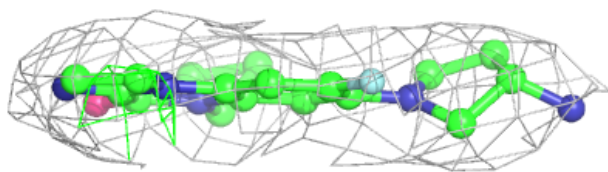
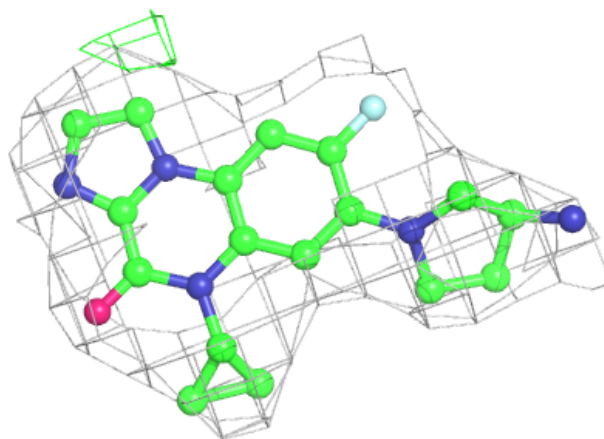
Electron density around E32 e 1001:

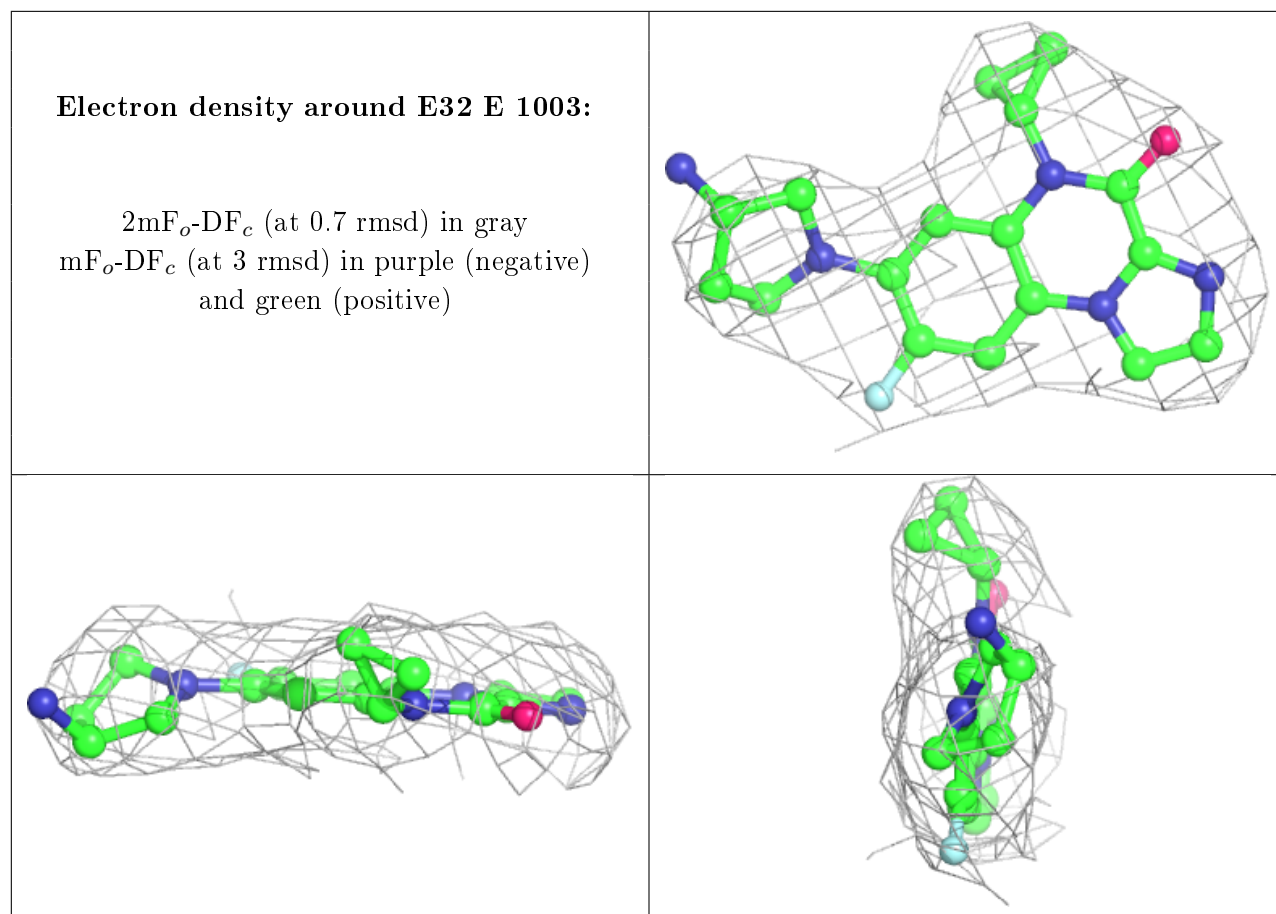
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around E32 E 1001:

$2mF_o-DF_c$ (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.