



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:12 pm BST

PDB ID : 6FQS  
Title : 3.11A complex of S.Aureus gyrase with imidazopyrazinone T3 and DNA  
Authors : Bax, B.D.; Germe, T.; Basque, E.; Maxwell, A.  
Deposited on : 2018-02-14  
Resolution : 3.11 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.11  
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) : 2.11

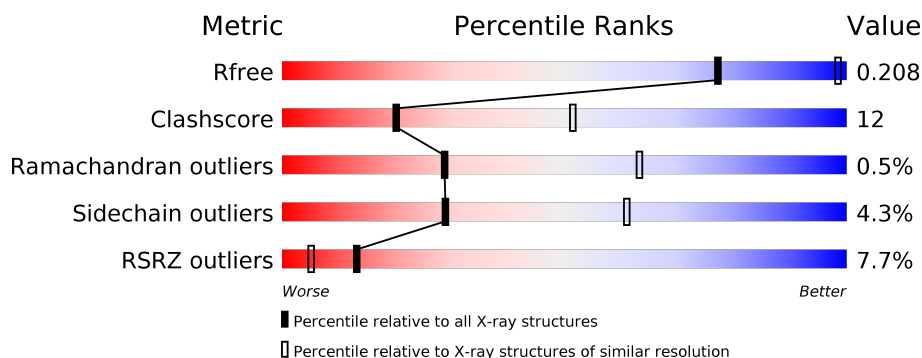
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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  $\geq 3$ , 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	202	<div> <div>27%</div> <div>65%</div> <div>22%</div> <div>6%</div> <div>6%</div> </div>
1	D	202	<div> <div>25%</div> <div>67%</div> <div>24%</div> <div>6%</div> </div>
2	A	490	<div> <div>77%</div> <div>20%</div> <div>3%</div> </div>
3	C	490	<div> <div>80%</div> <div>17%</div> <div>3%</div> </div>
4	E	20	<div> <div>35%</div> <div>40%</div> <div>25%</div> </div>
4	F	20	<div> <div>5%</div> <div>35%</div> <div>45%</div> <div>20%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	A	502	-	-	-	X
7	GOL	A	504	-	-	-	X
7	GOL	C	502	-	-	-	X
7	GOL	C	503	-	-	-	X
9	E3E	E	103[B]	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 11870 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	189	Total	C	N	O	S	0	4	0
			1464	920	252	284	8			
1	D	189	Total	C	N	O	S	0	2	0
			1466	922	252	282	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	LEU	conflict	UNP P66937
B	544	THR	-	linker	UNP P66937
B	579	GLY	-	linker	UNP P66937
D	409	MET	LEU	conflict	UNP P66937
D	544	THR	-	linker	UNP P66937
D	545	GLY	-	linker	UNP P66937

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	481	Total	C	N	O	S	0	6	0
			3883	2413	709	745	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	481	Total	C	N	O	P S	0	11	0
			3907	2421	708	759	1 18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	20	Total	C	N	O	P	0	3	0
			462	223	85	133	21			
4	F	20	Total	C	N	O	P	0	2	0
			448	215	81	131	21			

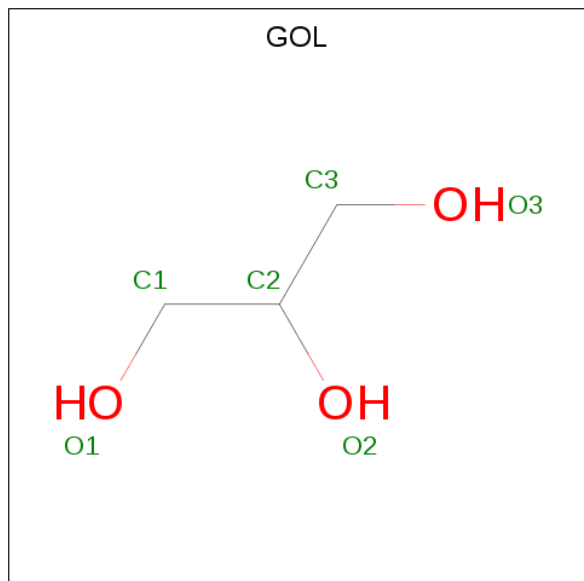
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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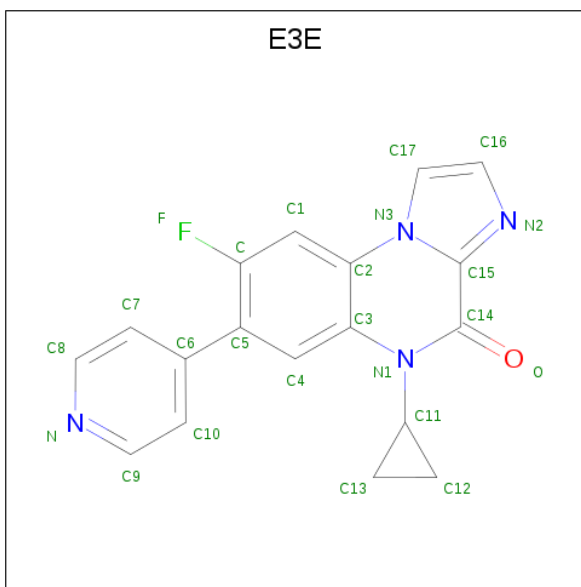
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 9 is 5-cyclopropyl-8-fluoranyl-7-pyridin-4-yl-imidazo[1,2-a]quinoxalin-4-one (three-letter code: E3E) (formula: C<sub>18</sub>H<sub>13</sub>FN<sub>4</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	F	N	O	0	0
			24	18	1	4	1		
9	E	1	Total	C	F	N	O	0	1
			48	36	2	8	2		

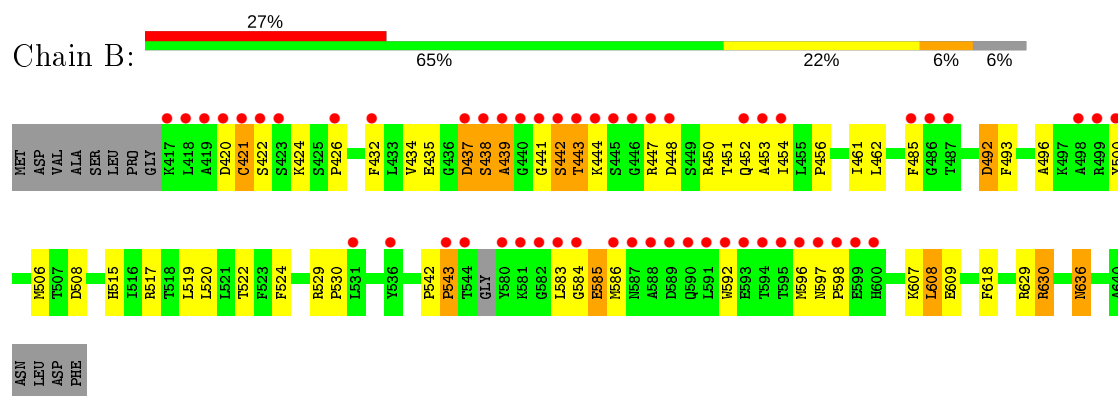
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	8	Total	O	0	0
			8	8		
10	A	46	Total	O	0	0
			46	46		
10	D	4	Total	O	0	0
			4	4		
10	C	39	Total	O	0	0
			39	39		
10	E	4	Total	O	0	0
			4	4		
10	F	11	Total	O	0	0
			11	11		

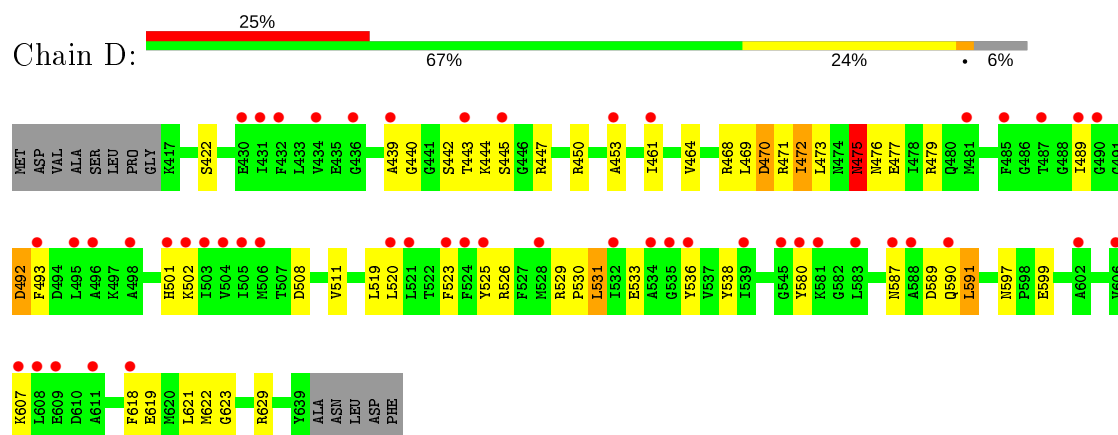
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

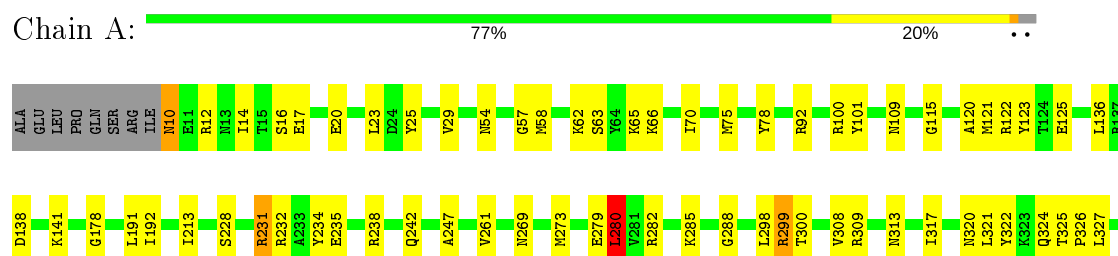
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B



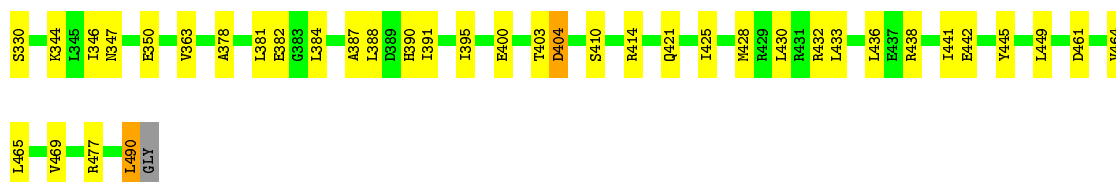
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B



- Molecule 2: DNA gyrase subunit A

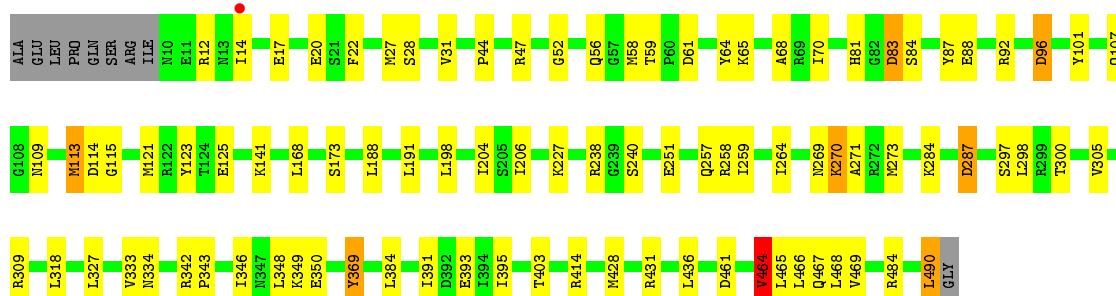






- Molecule 3: DNA gyrase subunit A

Chain C: 80% 17% ..



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

Chain E: 35% 40% 25%



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

Chain F: 5% 35% 45% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.03Å 94.03Å 420.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.01 – 3.11 48.34 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.01-3.11) 99.9 (48.34-3.11)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.179 , 0.210 0.179 , 0.208	Depositor DCC
$R_{free}$ test set	1843 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.0	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.078 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, NA, MN, E3E, SO4, PTR

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	0.49	0/1487	0.71	2/2014 (0.1%)
1	D	0.67	2/1490 (0.1%)	0.87	5/2017 (0.2%)
2	A	0.45	1/3932 (0.0%)	0.64	4/5295 (0.1%)
3	C	0.47	1/3937 (0.0%)	0.65	1/5301 (0.0%)
4	E	1.50	10/517 (1.9%)	1.30	3/794 (0.4%)
4	F	1.18	4/500 (0.8%)	1.37	4/766 (0.5%)
All	All	0.62	18/11863 (0.2%)	0.78	19/16187 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	477	GLU	CB-CG	-12.52	1.28	1.52
4	E	-4	DG	C3'-O3'	-11.39	1.29	1.44
4	E	1	DG	C3'-O3'	-9.20	1.31	1.44
3	C	464	VAL	CB-CG2	-7.54	1.37	1.52
1	D	475	ASN	CB-CG	7.42	1.68	1.51
4	F	-1[A]	DT	N1-C2	-7.41	1.32	1.38
4	F	-1[B]	DT	N1-C2	-7.41	1.32	1.38
4	E	5[A]	DA	N9-C4	-6.64	1.33	1.37
4	E	5[B]	DA	N9-C4	-6.64	1.33	1.37
4	E	5[A]	DA	C2-N3	-6.58	1.27	1.33
4	E	5[B]	DA	C2-N3	-6.58	1.27	1.33
4	E	-7	DA	C3'-O3'	-6.05	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	231	ARG	CB-CG	-5.81	1.36	1.52
4	E	5[A]	DA	N3-C4	-5.69	1.31	1.34
4	E	5[B]	DA	N3-C4	-5.69	1.31	1.34
4	E	-8	DG	N7-C5	-5.53	1.35	1.39
4	F	10	DC	C3'-O3'	-5.50	1.36	1.44
4	F	-8	DG	C3'-O3'	-5.46	1.36	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	475	ASN	N-CA-C	11.99	143.39	111.00
1	D	475	ASN	CB-CA-C	-9.39	91.62	110.40
1	D	475	ASN	CA-C-O	-9.06	101.07	120.10
2	A	280	LEU	CB-CG-CD1	-8.82	96.01	111.00
1	B	508	ASP	CB-CG-OD2	-8.05	111.06	118.30
4	F	-2	DA	P-O3'-C3'	7.99	129.29	119.70
4	E	2	DG	OP1-P-OP2	-7.30	108.65	119.60
1	D	508	ASP	CB-CG-OD2	-7.17	111.84	118.30
4	F	12	DT	C1'-O4'-C4'	-7.12	102.98	110.10
1	B	608	LEU	C-N-CA	-6.55	105.32	121.70
4	E	1	DG	OP2-P-O3'	6.29	119.03	105.20
4	F	-2	DA	OP1-P-O3'	6.13	118.68	105.20
1	D	475	ASN	O-C-N	6.04	132.36	122.70
2	A	490	LEU	CA-CB-CG	5.62	128.23	115.30
2	A	121	MET	CA-CB-CG	5.51	122.67	113.30
4	F	12	DT	O4'-C1'-N1	5.46	111.82	108.00
3	C	284	LYS	CD-CE-NZ	5.43	124.19	111.70
4	E	-6	DG	O5'-P-OP1	-5.09	101.12	105.70
2	A	430	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	439[B]	ALA	Peptide

## 5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1464	0	1398	68	0
1	D	1466	0	1411	42	0
2	A	3883	0	3928	82	0
3	C	3907	0	3914	76	0
4	E	462	0	257	30	0
4	F	448	0	246	30	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
7	A	24	0	32	1	0
7	C	18	0	24	3	0
7	E	6	0	8	2	0
8	C	5	0	0	0	0
9	E	72	0	0	12	0
10	A	46	0	0	0	0
10	B	8	0	0	0	0
10	C	39	0	0	0	0
10	D	4	0	0	0	0
10	E	4	0	0	2	0
10	F	11	0	0	1	0
All	All	11870	0	11218	286	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (286) 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)
4:F:3:DC:H2''	4:F:4:DC:H5'	1.25	1.17
4:E:5[A]:DA:N1	4:F:-1[A]:DT:N3	1.94	1.16
2:A:321:LEU:O	2:A:325:THR:OG1	1.63	1.15
1:B:447:ARG:NH2	1:B:452:GLN:O	1.79	1.14
1:B:438[B]:SER:HA	1:B:441:GLY:HA3	1.30	1.08
3:C:56:GLN:OE1	3:C:65:LYS:NZ	1.86	1.07
4:F:-2:DA:H2''	4:F:-1[A]:DT:H5'	1.38	1.05
4:F:11:DT:H2''	4:F:12:DT:H4'	1.56	0.88
1:D:493:PHE:CE2	1:D:530:PRO:HB2	2.09	0.87
3:C:204:ILE:O	3:C:349:LYS:NZ	2.06	0.86
4:E:-4:DG:N7	7:E:101:GOL:O2	2.08	0.84
1:D:531:LEU:HD11	1:D:536:TYR:HB2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:-5:DA:N7	7:E:101:GOL:O3	2.10	0.84
3:C:12:ARG:NH2	3:C:20:GLU:OE2	2.10	0.84
2:A:438:ARG:HH12	2:A:442:GLU:HB2	1.45	0.80
2:A:122[A]:ARG:NH2	4:F:1[A]:DG:H5"	1.98	0.79
1:B:438[B]:SER:HA	1:B:441:GLY:CA	2.11	0.78
2:A:438:ARG:NH1	2:A:438:ARG:O	2.17	0.78
4:F:8:DC:H2"	4:F:9:DT:H5"	1.66	0.77
2:A:231:ARG:O	2:A:235[A]:GLU:HG3	1.84	0.76
1:B:420:ASP:OD1	1:B:500:TYR:OH	2.04	0.76
1:B:592:TRP:HA	1:B:596:MET:HB2	1.68	0.76
3:C:227:LYS:HD2	3:C:490:LEU:HD21	1.67	0.76
1:B:437[B]:ASP:HB2	4:E:2:DG:P	2.26	0.76
2:A:122[B]:ARG:NH2	2:A:123[B]:TYR:OH	2.16	0.75
1:D:629:ARG:HD2	3:C:22:PHE:HZ	1.50	0.74
3:C:84:SER:O	3:C:88:GLU:HG3	1.87	0.74
3:C:83:ASP:OD1	3:C:83:ASP:N	2.18	0.73
3:C:68:ALA:HA	3:C:121:MET:HE3	1.71	0.73
1:B:515:HIS:HB2	2:A:25:TYR:CD1	2.22	0.73
2:A:432:ARG:HH11	2:A:432:ARG:HG3	1.52	0.72
4:E:5[A]:DA:N6	4:F:-1[A]:DT:O4	2.15	0.71
1:B:437[A]:ASP:N	1:B:437[A]:ASP:OD1	2.22	0.71
4:F:-2:DA:C2'	4:F:-1[A]:DT:H5'	2.17	0.71
3:C:64:TYR:HB3	3:C:125:GLU:HB3	1.73	0.71
3:C:58:MET:HE1	3:C:65:LYS:HB2	1.72	0.70
2:A:308:VAL:HG13	2:A:317:ILE:HD12	1.72	0.69
2:A:320:ASN:O	2:A:324:GLN:HG3	1.94	0.68
3:C:58:MET:CE	3:C:65:LYS:HB2	2.23	0.68
1:D:531:LEU:O	1:D:531:LEU:HD12	1.93	0.68
2:A:404:ASP:OD2	3:C:431:ARG:NH1	2.26	0.67
1:D:475:ASN:O	1:D:475:ASN:CG	2.34	0.66
1:B:444:LYS:HA	1:B:447:ARG:HD3	1.78	0.66
2:A:391:ILE:HD11	2:A:395:ILE:HD11	1.78	0.66
1:B:592:TRP:HA	1:B:596:MET:CB	2.25	0.66
2:A:16:SER:O	2:A:20:GLU:HG3	1.95	0.65
1:B:585:GLU:N	1:B:585:GLU:OE2	2.28	0.65
3:C:68:ALA:HA	3:C:121:MET:CE	2.26	0.65
2:A:54:ASN:HB2	2:A:136:LEU:HD13	1.77	0.65
1:D:461:ILE:O	1:D:519:LEU:HD13	1.97	0.65
4:F:-3:DT:H2"	4:F:-2:DA:H5"	1.79	0.65
3:C:47:ARG:HH11	7:C:502:GOL:H31	1.62	0.64
4:E:4[B]:DC:H2'	9:E:103[B]:E3E:C10	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437[B]:ASP:HB2	4:E:2:DG:OP1	1.98	0.64
4:F:1[A]:DG:H2'	4:F:2:DG:C8	2.33	0.63
1:B:443:THR:O	1:B:447:ARG:N	2.23	0.63
2:A:387:ALA:HB2	2:A:425:ILE:HD13	1.80	0.63
3:C:309:ARG:HG2	3:C:309:ARG:HH11	1.63	0.63
3:C:466:LEU:O	3:C:469:VAL:N	2.32	0.63
4:E:5[B]:DA:C8	9:E:103[B]:E3E:C10	2.81	0.63
4:E:-8:DG:N7	4:F:12:DT:C7	2.62	0.63
4:F:-2:DA:H2''	4:F:-1[A]:DT:C5'	2.23	0.63
4:E:5[A]:DA:H2	4:F:-1[A]:DT:O2	1.82	0.62
3:C:461:ASP:HB3	3:C:464:VAL:CG2	2.30	0.62
1:B:522:THR:HA	1:B:618:PHE:CE1	2.35	0.62
2:A:344:LYS:NZ	2:A:350:GLU:OE2	2.21	0.62
1:B:438[B]:SER:C	1:B:441:GLY:H	2.03	0.62
2:A:122[B]:ARG:NH2	4:F:1[B]:DG:H5''	2.14	0.62
1:D:476[B]:ASN:OD1	1:D:479:ARG:NH2	2.23	0.61
3:C:107:GLN:HB3	3:C:125:GLU:HB2	1.83	0.61
4:E:11:DT:H1'	10:E:201:HOH:O	2.01	0.60
1:D:493:PHE:CD2	1:D:530:PRO:HG2	2.36	0.60
2:A:384:LEU:HD22	2:A:428:MET:HE2	1.83	0.60
4:E:-8:DG:N7	4:F:12:DT:H73	2.17	0.60
4:E:5[B]:DA:N7	9:E:103[B]:E3E:C10	2.65	0.60
2:A:58:MET:SD	2:A:65:LYS:HB2	2.41	0.59
1:D:439:ALA:O	1:D:443:THR:HG23	2.02	0.59
1:B:515:HIS:HB2	2:A:25:TYR:CG	2.37	0.59
2:A:432:ARG:HG3	2:A:432:ARG:NH1	2.15	0.59
3:C:59:THR:OG1	3:C:61:ASP:OD1	2.15	0.59
2:A:273:MET:SD	2:A:327:LEU:HD12	2.42	0.59
3:C:113:MET:HE2	3:C:264:ILE:HD11	1.85	0.58
2:A:465:LEU:HD12	2:A:465:LEU:O	2.03	0.58
3:C:287[B]:ASP:OD1	3:C:287[B]:ASP:N	2.32	0.58
1:B:506:MET:HG2	1:B:583:LEU:HD11	1.86	0.57
1:B:592:TRP:HE3	1:B:596:MET:HG2	1.69	0.57
2:A:280:LEU:HD22	2:A:285:LYS:HB2	1.86	0.57
1:B:437[B]:ASP:HB2	4:E:1:DG:O3'	2.04	0.57
2:A:247:ALA:HB2	2:A:261:VAL:HG22	1.86	0.56
1:D:493:PHE:HE2	1:D:530:PRO:HB2	1.65	0.56
2:A:298:LEU:HD23	2:A:298:LEU:N	2.20	0.56
3:C:297:SER:HG	3:C:300:THR:H	1.52	0.56
3:C:96:ASP:OD1	3:C:96:ASP:N	2.32	0.56
2:A:461:ASP:HB3	2:A:464:VAL:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437[B]:ASP:O	1:B:438[B]:SER:HB2	2.05	0.56
1:D:629:ARG:HD2	3:C:22:PHE:CZ	2.36	0.56
3:C:461:ASP:HB3	3:C:464:VAL:HG23	1.87	0.56
1:D:619:GLU:O	1:D:623:GLY:HA3	2.06	0.56
1:B:592:TRP:CE3	1:B:596:MET:HB3	2.41	0.56
4:E:4[B]:DC:H3'	9:E:103[B]:E3E:C9	2.36	0.56
1:D:469:LEU:HA	1:D:472:ILE:HG13	1.87	0.56
1:B:439[A]:ALA:HB1	1:B:583:LEU:HB3	1.88	0.56
2:A:410:SER:O	2:A:414:ARG:HG2	2.05	0.55
2:A:57:GLY:O	2:A:62:LYS:HD2	2.06	0.55
1:D:476[A]:ASN:H	1:D:479:ARG:HG3	1.72	0.55
2:A:12:ARG:NE	2:A:17:GLU:OE1	2.25	0.55
2:A:384:LEU:HD22	2:A:428:MET:CE	2.36	0.55
4:E:2:DG:H2'	4:E:3[B]:DC:C6	2.41	0.55
3:C:47:ARG:HD2	7:C:502:GOL:H31	1.88	0.55
1:D:443:THR:O	1:D:447:ARG:HG2	2.07	0.55
1:D:501:HIS:O	1:D:536:TYR:HB3	2.07	0.55
4:E:2:DG:H2''	4:E:3[A]:DC:H5'	1.89	0.54
4:F:9:DT:H6	4:F:9:DT:H5'	1.71	0.54
1:B:432:PHE:HB2	1:B:454:ILE:HD13	1.89	0.54
4:E:5[A]:DA:C2	4:F:-1[A]:DT:O2	2.61	0.54
2:A:445:TYR:CE2	2:A:449:LEU:HD11	2.43	0.54
3:C:58:MET:SD	3:C:65:LYS:HD2	2.47	0.54
2:A:122[B]:ARG:NE	2:A:123[B]:TYR:CE1	2.76	0.53
1:B:444:LYS:HA	1:B:447:ARG:CD	2.38	0.53
1:D:422:SER:HB2	1:D:450:ARG:HA	1.90	0.53
2:A:378:ALA:O	2:A:382:GLU:HG3	2.09	0.53
3:C:52:GLY:O	3:C:56:GLN:HG3	2.09	0.53
1:D:502:LYS:HG2	1:D:538:TYR:CE1	2.44	0.53
3:C:81:HIS:HD1	4:F:-1[A]:DT:P	2.31	0.53
1:B:585:GLU:HB3	3:C:125:GLU:HG2	1.91	0.53
4:E:2:DG:H2'	4:E:3[A]:DC:C6	2.43	0.53
1:B:585:GLU:HB3	3:C:125:GLU:CG	2.39	0.53
3:C:393:GLU:OE2	3:C:414:ARG:NH1	2.30	0.52
1:B:437[A]:ASP:HA	1:B:456:PRO:HB2	1.90	0.52
2:A:58:MET:HE3	2:A:58:MET:HA	1.91	0.52
2:A:387:ALA:HB2	2:A:425:ILE:CD1	2.40	0.52
1:B:437[B]:ASP:O	4:E:2:DG:OP1	2.28	0.52
1:D:587:ASN:HD22	1:D:590:GLN:CD	2.12	0.52
4:E:4[B]:DC:C5	9:E:103[B]:E3E:C8	2.93	0.52
1:B:438[B]:SER:CA	1:B:441:GLY:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:ASP:N	1:B:492:ASP:OD1	2.42	0.51
2:A:109:ASN:HB2	1:D:442:SER:OG	2.11	0.51
2:A:299:ARG:N	2:A:299:ARG:HD3	2.26	0.51
1:D:618:PHE:HZ	3:C:14:ILE:HD11	1.75	0.51
4:F:3:DC:C2'	4:F:4:DC:H5'	2.18	0.51
1:D:440:GLY:O	1:D:444:LYS:HG3	2.11	0.50
1:B:542:PRO:CB	1:B:543:PRO:HD2	2.42	0.50
1:B:485:PHE:HE2	1:B:524:PHE:HE1	1.59	0.50
1:D:597:ASN:OD1	1:D:599:GLU:HG3	2.11	0.50
2:A:191:LEU:HD23	2:A:213:ILE:HD13	1.92	0.50
1:B:585:GLU:HA	3:C:123:PTR:O	2.11	0.50
3:C:114:ASP:HB3	3:C:271:ALA:HB2	1.93	0.50
1:D:529:ARG:N	1:D:530:PRO:HD2	2.26	0.50
2:A:421:GLN:O	2:A:425:ILE:HG13	2.12	0.50
3:C:123:PTR:O2P	3:C:123:PTR:HE1	2.12	0.49
1:B:608:LEU:HA	2:A:14:ILE:HG22	1.93	0.49
2:A:313:ASN:O	2:A:317:ILE:HG13	2.13	0.49
4:E:4[B]:DC:C5	9:E:103[B]:E3E:C7	2.96	0.49
1:D:618:PHE:CZ	3:C:14:ILE:HD11	2.47	0.49
3:C:27[B]:MET:O	3:C:31:VAL:HG22	2.12	0.49
1:D:476[B]:ASN:H	1:D:479:ARG:HG3	1.76	0.49
2:A:279[B]:GLU:HG2	2:A:282:ARG:NH1	2.28	0.49
3:C:238:ARG:HD2	3:C:334:ASN:OD1	2.13	0.49
1:D:519:LEU:HD23	1:D:622:MET:CE	2.43	0.49
2:A:100:ARG:HG3	2:A:101:TYR:CE2	2.47	0.49
1:D:461:ILE:HD13	1:D:520:LEU:HD23	1.95	0.48
1:B:608:LEU:HD12	1:B:609:GLU:N	2.28	0.48
4:E:5[A]:DA:C2	4:F:-1[A]:DT:N3	2.76	0.48
3:C:259:ILE:HG21	3:C:318:LEU:HD13	1.95	0.48
2:A:238:ARG:HD3	10:F:108:HOH:O	2.13	0.48
2:A:346:ILE:HB	2:A:350:GLU:HB3	1.95	0.48
1:B:437[B]:ASP:CB	4:E:2:DG:OP1	2.61	0.48
4:E:5[B]:DA:H2	4:F:-1[B]:DT:O2	1.97	0.48
1:B:529:ARG:N	1:B:530:PRO:HD2	2.28	0.48
3:C:87:TYR:CD1	3:C:121:MET:HG2	2.49	0.48
3:C:461:ASP:CB	3:C:464:VAL:HG23	2.44	0.47
2:A:325:THR:HB	2:A:326:PRO:CD	2.44	0.47
1:B:608:LEU:C	1:B:608:LEU:HD12	2.34	0.47
3:C:101:TYR:CZ	3:C:188:LEU:HB2	2.49	0.47
3:C:27[A]:MET:O	3:C:31:VAL:HG22	2.13	0.47
1:B:432:PHE:HB2	1:B:454:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ILE:O	1:B:519:LEU:HD13	2.14	0.47
4:E:5[A]:DA:C2	4:F:-1[A]:DT:C2	3.03	0.47
2:A:436:LEU:HD12	3:C:403:THR:HG22	1.97	0.47
1:D:470:ASP:HA	1:D:473:LEU:HD12	1.95	0.47
9:E:103[B]:E3E:C4	9:E:103[B]:E3E:C13	2.93	0.47
2:A:122[B]:ARG:HH21	4:F:1[B]:DG:H5''	1.79	0.47
1:D:511:VAL:HG11	3:C:28:SER:HB2	1.96	0.47
3:C:465:LEU:HD12	3:C:465:LEU:O	2.15	0.47
9:E:103[A]:E3E:C12	9:E:103[A]:E3E:C4	2.92	0.47
9:E:103[B]:E3E:C4	9:E:103[B]:E3E:C12	2.92	0.47
9:E:103[A]:E3E:C4	9:E:103[A]:E3E:C13	2.93	0.47
4:E:7:DA:H2''	4:E:8:DC:H5'	1.96	0.47
2:A:322:TYR:CE1	2:A:327:LEU:HD23	2.49	0.47
3:C:273:MET:SD	3:C:327:LEU:HD13	2.55	0.47
1:D:493:PHE:CD2	1:D:530:PRO:HB2	2.48	0.47
2:A:404:ASP:OD1	2:A:404:ASP:N	2.47	0.47
1:B:584:GLY:O	1:B:586:MET:N	2.47	0.47
4:E:4[B]:DC:H2'	9:E:103[B]:E3E:C9	2.45	0.47
1:B:522:THR:HA	1:B:618:PHE:HE1	1.79	0.46
3:C:238:ARG:HA	3:C:333:VAL:O	2.15	0.46
3:C:342:ARG:HB2	3:C:343:PRO:HD2	1.96	0.46
2:A:115:GLY:HA3	2:A:269:ASN:ND2	2.31	0.46
3:C:258:ARG:HD2	3:C:305:VAL:HG13	1.97	0.46
3:C:264:ILE:HD13	3:C:270:LYS:HG3	1.97	0.46
2:A:403:THR:HG22	3:C:436:LEU:HD22	1.97	0.46
3:C:65:LYS:HD3	3:C:70:ILE:HG12	1.95	0.46
1:B:584:GLY:HA2	3:C:123:PTR:HD1	1.97	0.46
3:C:56:GLN:HE22	3:C:70:ILE:HA	1.79	0.46
1:B:493:PHE:CD1	1:B:493:PHE:C	2.89	0.46
2:A:12:ARG:HH22	2:A:20:GLU:CD	2.19	0.46
1:B:438[B]:SER:CA	1:B:441:GLY:CA	2.90	0.46
4:F:-8:DG:N3	4:F:-8:DG:C2'	2.78	0.45
2:A:308:VAL:HG13	2:A:317:ILE:CD1	2.42	0.45
3:C:348:LEU:HG	3:C:348:LEU:O	2.16	0.45
2:A:10:ASN:N	2:A:10:ASN:ND2	2.65	0.45
2:A:234:TYR:O	2:A:347:ASN:HB2	2.16	0.45
2:A:58:MET:CE	2:A:65:LYS:HB2	2.47	0.45
1:D:621:LEU:HD22	3:C:22:PHE:CD2	2.51	0.45
2:A:120:ALA:HB3	2:A:123[A]:TYR:CE2	2.52	0.45
1:D:442:SER:HB3	1:D:591:LEU:HD23	1.98	0.45
1:B:542:PRO:HB3	1:B:543:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:384:LEU:HD22	3:C:428:MET:HE2	1.98	0.45
3:C:461:ASP:HB3	3:C:464:VAL:HG21	1.96	0.45
1:D:464:VAL:HG21	1:D:523:PHE:HA	1.99	0.45
1:B:434:VAL:HA	1:B:506:MET:O	2.17	0.45
1:D:531:LEU:CD1	1:D:536:TYR:HB2	2.41	0.45
1:D:470:ASP:OD1	1:D:471:ARG:N	2.50	0.44
2:A:388:LEU:HD23	2:A:388:LEU:HA	1.82	0.44
2:A:138:ASP:H	7:A:503:GOL:H2	1.83	0.44
2:A:122[A]:ARG:HH21	4:F:1[A]:DG:P	2.40	0.44
1:B:453:ALA:O	1:B:454:ILE:HD13	2.16	0.44
1:B:585:GLU:H	1:B:585:GLU:CD	2.05	0.44
3:C:198:LEU:O	3:C:198:LEU:HD12	2.18	0.44
3:C:391:ILE:O	3:C:395:ILE:HG12	2.18	0.44
3:C:191:LEU:HD23	3:C:191:LEU:HA	1.80	0.44
2:A:363:VAL:HG21	2:A:469:VAL:HG22	2.00	0.43
3:C:466:LEU:O	3:C:467:GLN:C	2.55	0.43
2:A:381:LEU:HD22	2:A:441:ILE:HG23	2.00	0.43
1:B:438[B]:SER:C	1:B:441:GLY:N	2.70	0.43
1:B:437[A]:ASP:HA	1:B:456:PRO:CB	2.49	0.43
1:B:443:THR:HB	1:B:596:MET:CE	2.48	0.43
1:B:607:LYS:O	2:A:14:ILE:N	2.49	0.43
3:C:257:GLN:HG3	7:C:503:GOL:H12	2.00	0.43
2:A:92:ARG:HD2	10:E:203:HOH:O	2.18	0.43
1:B:597:ASN:HA	1:B:598:PRO:HD3	1.85	0.43
1:B:448:ASP:O	1:B:452:GLN:HB2	2.19	0.43
1:B:520:LEU:HA	1:B:520:LEU:HD23	1.82	0.43
3:C:168:LEU:HD23	3:C:168:LEU:HA	1.70	0.43
1:B:424:LYS:O	1:B:426:PRO:HD3	2.19	0.43
2:A:122[A]:ARG:HH22	4:F:1[A]:DG:H5"	1.78	0.43
2:A:242:GLN:NE2	2:A:330:SER:HB2	2.34	0.43
1:B:437[A]:ASP:O	1:B:441:GLY:N	2.52	0.43
3:C:346:ILE:HB	3:C:350:GLU:HB2	2.01	0.43
4:E:5[B]:DA:C2	4:F:-1[B]:DT:O2	2.71	0.43
2:A:66:LYS:HA	2:A:125:GLU:HG2	2.00	0.42
1:D:468:ARG:NH2	1:D:470:ASP:OD2	2.52	0.42
9:E:103[B]:E3E:N2	4:F:-1[B]:DT:H2'	2.34	0.42
1:B:437[B]:ASP:CB	4:E:2:DG:P	3.01	0.42
2:A:23:LEU:HD12	2:A:23:LEU:HA	1.78	0.42
2:A:322:TYR:CD1	2:A:327:LEU:HD23	2.54	0.42
1:D:492:ASP:OD1	1:D:492:ASP:N	2.53	0.42
1:B:443:THR:HB	1:B:596:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:381:LEU:HD23	2:A:381:LEU:HA	1.85	0.42
3:C:466:LEU:O	3:C:468:LEU:N	2.52	0.42
2:A:438:ARG:HA	2:A:438:ARG:HD2	1.80	0.42
2:A:58:MET:HE1	2:A:65:LYS:HB2	2.01	0.42
1:B:442:SER:HA	3:C:109:ASN:HB2	2.02	0.42
3:C:369:TYR:CD1	3:C:369:TYR:C	2.92	0.42
2:A:288:GLY:HA2	2:A:309:ARG:NH1	2.35	0.42
2:A:25:TYR:CE2	2:A:29:VAL:HG21	2.55	0.42
3:C:64:TYR:HB3	3:C:125:GLU:CB	2.46	0.41
1:B:461:ILE:O	1:B:462:LEU:C	2.59	0.41
1:B:596:MET:HE2	1:B:596:MET:HB2	1.84	0.41
1:B:629:ARG:NE	4:F:9:DT:OP1	2.53	0.41
3:C:17:GLU:OE1	3:C:17:GLU:HA	2.20	0.41
1:D:530:PRO:HA	1:D:533:GLU:OE2	2.20	0.41
2:A:300:THR:O	2:A:300:THR:HG22	2.18	0.41
3:C:92[B]:ARG:NH1	4:F:-3:DT:OP2	2.52	0.41
1:D:607:LYS:O	3:C:14:ILE:HG22	2.21	0.41
2:A:192:ILE:HG21	2:A:477:ARG:HB2	2.03	0.41
1:B:421:CYS:HB2	1:B:450:ARG:O	2.20	0.41
2:A:465:LEU:HD12	2:A:465:LEU:C	2.40	0.41
3:C:115:GLY:HA3	3:C:269:ASN:ND2	2.36	0.41
1:B:630:ARG:HB2	2:A:178:GLY:O	2.21	0.41
1:B:517:ARG:NE	2:A:17:GLU:OE2	2.54	0.41
1:D:447:ARG:NH2	1:D:453:ALA:HA	2.36	0.40
1:B:636:ASN:HD22	1:B:636:ASN:N	2.19	0.40
3:C:92[A]:ARG:HH11	3:C:92[A]:ARG:HD3	1.69	0.40
1:D:525:TYR:HE1	1:D:526:ARG:NH1	2.19	0.40
2:A:66:LYS:O	2:A:70:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	189/202 (94%)	176 (93%)	10 (5%)	3 (2%)	9	36
1	D	189/202 (94%)	182 (96%)	6 (3%)	1 (0%)	29	63
2	A	485/490 (99%)	472 (97%)	12 (2%)	1 (0%)	47	79
3	C	489/490 (100%)	474 (97%)	14 (3%)	1 (0%)	47	79
All	All	1352/1384 (98%)	1304 (96%)	42 (3%)	6 (0%)	29	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	470	ASP
2	A	141	LYS
1	B	443	THR
1	B	496	ALA
1	B	543	PRO
3	C	141	LYS

### 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	147/168 (88%)	134 (91%)	13 (9%)	10	35
1	D	150/168 (89%)	141 (94%)	9 (6%)	19	49
2	A	421/423 (100%)	407 (97%)	14 (3%)	38	68
3	C	422/422 (100%)	406 (96%)	16 (4%)	33	65
All	All	1140/1181 (96%)	1088 (95%)	52 (5%)	29	59

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

Mol	Chain	Res	Type
1	B	421	CYS
1	B	422	SER
1	B	435	GLU
1	B	437[A]	ASP
1	B	437[B]	ASP

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Mol	Chain	Res	Type
1	B	438[A]	SER
1	B	438[B]	SER
1	B	442	SER
1	B	451	THR
1	B	492	ASP
1	B	585	GLU
1	B	630	ARG
1	B	636	ASN
2	A	10	ASN
2	A	63	SER
2	A	75	MET
2	A	78	TYR
2	A	228	SER
2	A	232[A]	ARG
2	A	232[B]	ARG
2	A	280	LEU
2	A	299	ARG
2	A	390	HIS
2	A	400	GLU
2	A	404	ASP
2	A	433	LEU
2	A	490	LEU
1	D	445	SER
1	D	472	ILE
1	D	475	ASN
1	D	489	ILE
1	D	492	ASP
1	D	531	LEU
1	D	580	TYR
1	D	589	ASP
1	D	591	LEU
3	C	44	PRO
3	C	83	ASP
3	C	96	ASP
3	C	113	MET
3	C	173	SER
3	C	206	ILE
3	C	240	SER
3	C	251	GLU
3	C	270	LYS
3	C	287[A]	ASP
3	C	287[B]	ASP

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Mol	Chain	Res	Type
3	C	298	LEU
3	C	369	TYR
3	C	464	VAL
3	C	484	ARG
3	C	490	LEU

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

Mol	Chain	Res	Type
2	A	10	ASN
2	A	446	ASN
1	D	474	ASN
1	D	587	ASN
1	D	590	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PTR	C	123	3,4	15,16,17	1.32	1 (6%)	19,22,24	1.00	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
3	PTR	C	123	3,4	-	1/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	123	PTR	OH-CZ	-4.24	1.31	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	123	PTR	CB-CA-C	-3.46	104.97	111.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	123	PTR	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	123	PTR	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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
9	E3E	E	103[B]	-	23,28,28	0.88	1 (4%)	21,42,42	1.21	2 (9%)
7	GOL	A	503	-	5,5,5	0.29	0	5,5,5	0.36	0
7	GOL	C	503	-	5,5,5	0.34	0	5,5,5	0.19	0
7	GOL	A	502	-	5,5,5	0.37	0	5,5,5	0.24	0
7	GOL	C	502	-	5,5,5	0.42	0	5,5,5	0.50	0
7	GOL	A	505	-	5,5,5	0.25	0	5,5,5	0.44	0
7	GOL	E	101	-	5,5,5	0.33	0	5,5,5	0.42	0
7	GOL	C	504	-	5,5,5	0.35	0	5,5,5	0.25	0
9	E3E	E	102	-	23,28,28	0.65	1 (4%)	21,42,42	1.01	1 (4%)
7	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.52	0
9	E3E	E	103[A]	-	23,28,28	0.82	1 (4%)	21,42,42	1.02	1 (4%)
8	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.09	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
9	E3E	E	103[B]	-	-	6/8/10/10	0/5/5/5
7	GOL	A	503	-	-	0/4/4/4	-
7	GOL	C	503	-	-	4/4/4/4	-
7	GOL	A	502	-	-	0/4/4/4	-
7	GOL	C	502	-	-	2/4/4/4	-
7	GOL	A	505	-	-	2/4/4/4	-
7	GOL	E	101	-	-	1/4/4/4	-
7	GOL	C	504	-	-	0/4/4/4	-
9	E3E	E	102	-	-	2/8/10/10	0/5/5/5
7	GOL	A	504	-	-	3/4/4/4	-
9	E3E	E	103[A]	-	-	5/8/10/10	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	103[B]	E3E	C3-N1	3.58	1.43	1.39
9	E	103[A]	E3E	C3-N1	3.58	1.43	1.39
9	E	102	E3E	C3-N1	2.07	1.41	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	103[B]	E3E	C16-C17-N3	-3.29	104.12	106.83
9	E	102	E3E	C16-C17-N3	-2.95	104.40	106.83
9	E	103[A]	E3E	C14-N1-C3	-2.74	119.22	121.75
9	E	103[B]	E3E	C14-N1-C3	-2.48	119.46	121.75

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	E	103[B]	E3E	C13-C11-N1-C3
9	E	103[B]	E3E	C12-C11-N1-C3
7	C	503	GOL	O1-C1-C2-C3
9	E	103[A]	E3E	C13-C11-N1-C3
9	E	103[A]	E3E	C12-C11-N1-C3
7	A	505	GOL	O1-C1-C2-O2
9	E	102	E3E	C13-C11-N1-C14
9	E	102	E3E	C12-C11-N1-C14
7	A	504	GOL	O1-C1-C2-C3
9	E	103[B]	E3E	C4-C5-C6-C10
9	E	103[B]	E3E	C4-C5-C6-C7
7	C	502	GOL	O2-C2-C3-O3
7	A	504	GOL	O1-C1-C2-O2
7	C	503	GOL	C1-C2-C3-O3
7	C	502	GOL	C1-C2-C3-O3
7	A	505	GOL	O1-C1-C2-C3
7	C	503	GOL	O1-C1-C2-O2
9	E	103[A]	E3E	C4-C5-C6-C10
9	E	103[B]	E3E	C-C5-C6-C10
9	E	103[B]	E3E	C-C5-C6-C7
9	E	103[A]	E3E	C4-C5-C6-C7
7	C	503	GOL	O2-C2-C3-O3
9	E	103[A]	E3E	C-C5-C6-C10
7	E	101	GOL	O1-C1-C2-O2
7	A	504	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 18 short contacts:

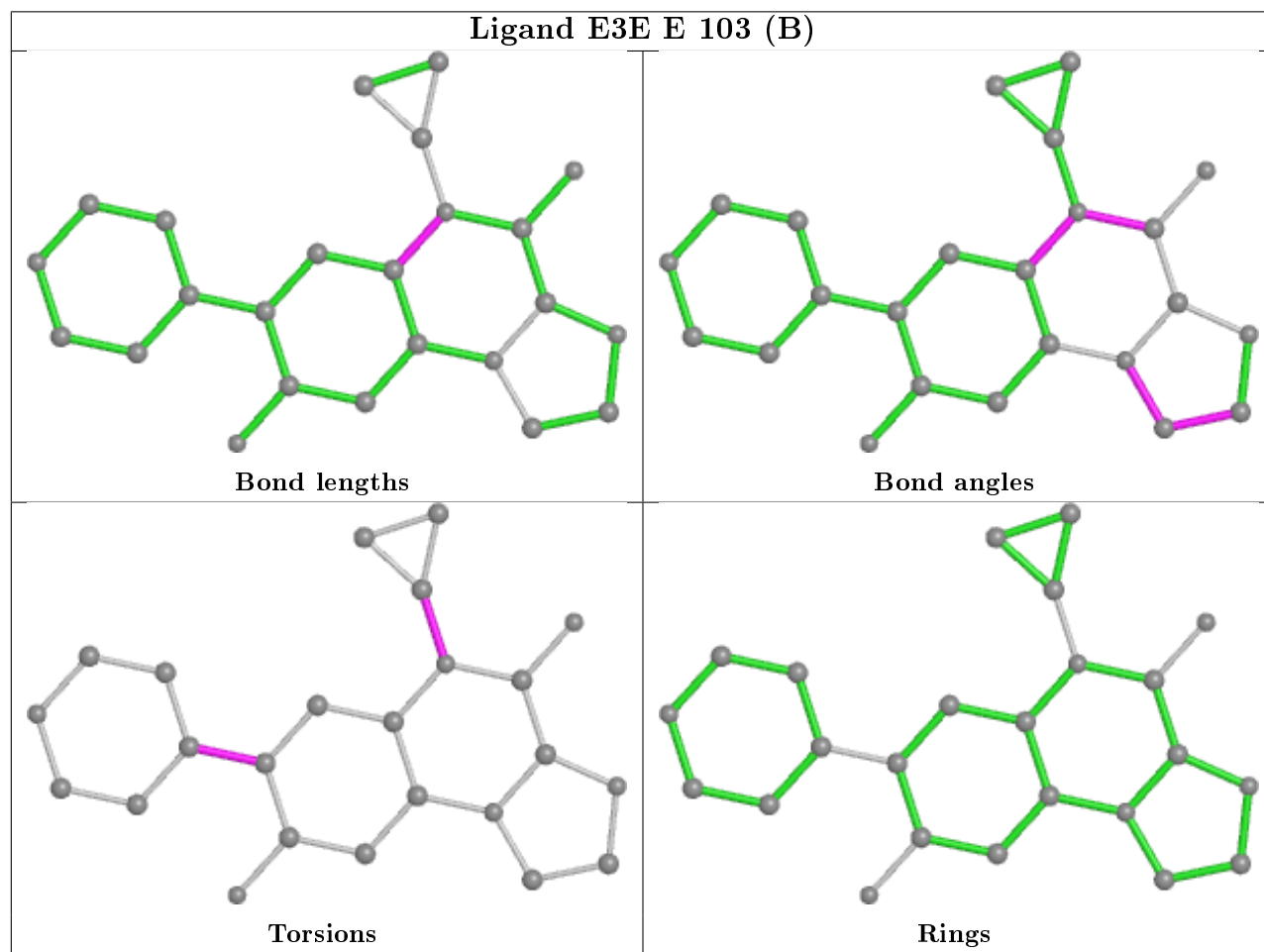
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	103[B]	E3E	10	0
7	A	503	GOL	1	0
7	C	503	GOL	1	0

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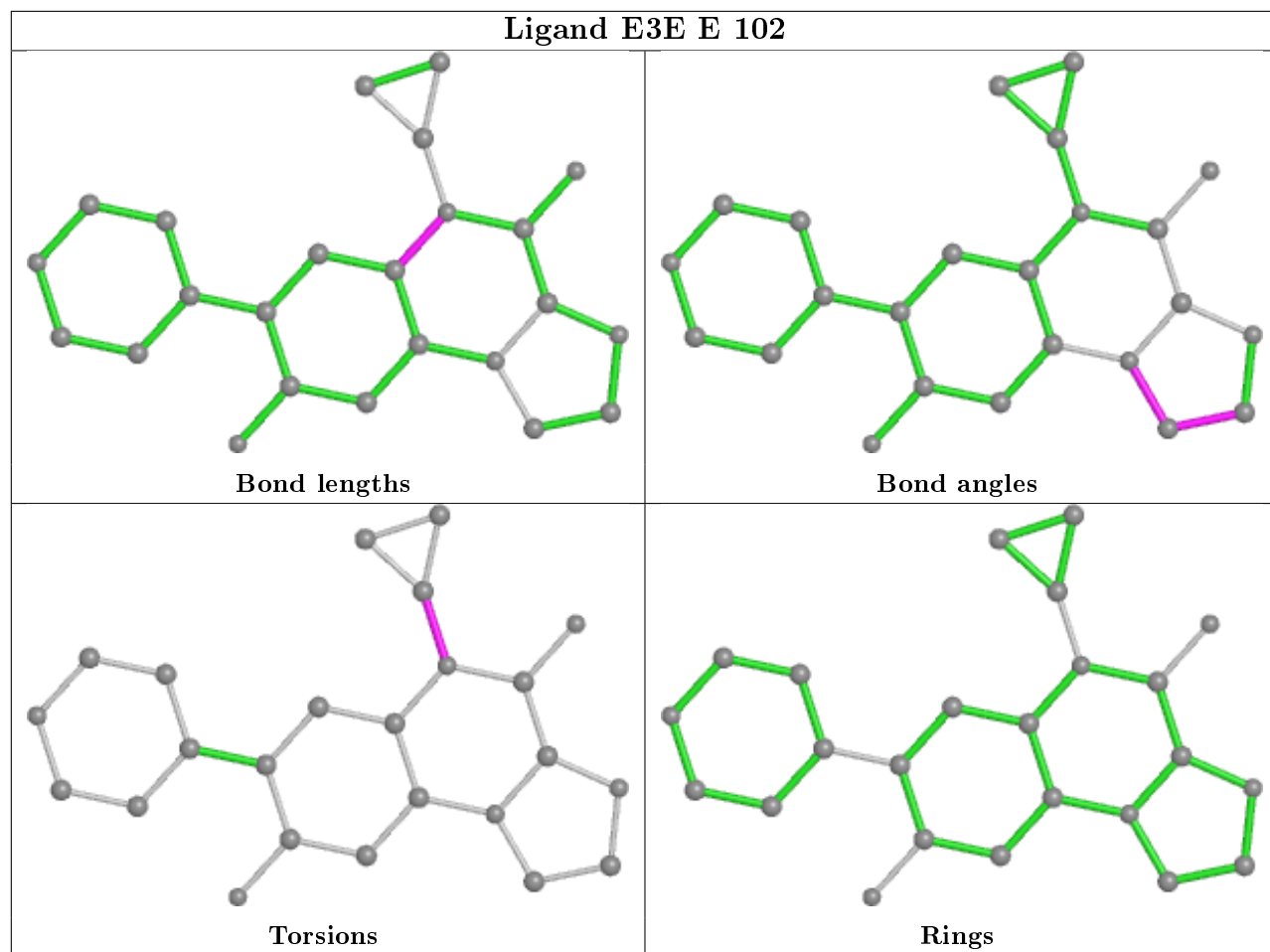
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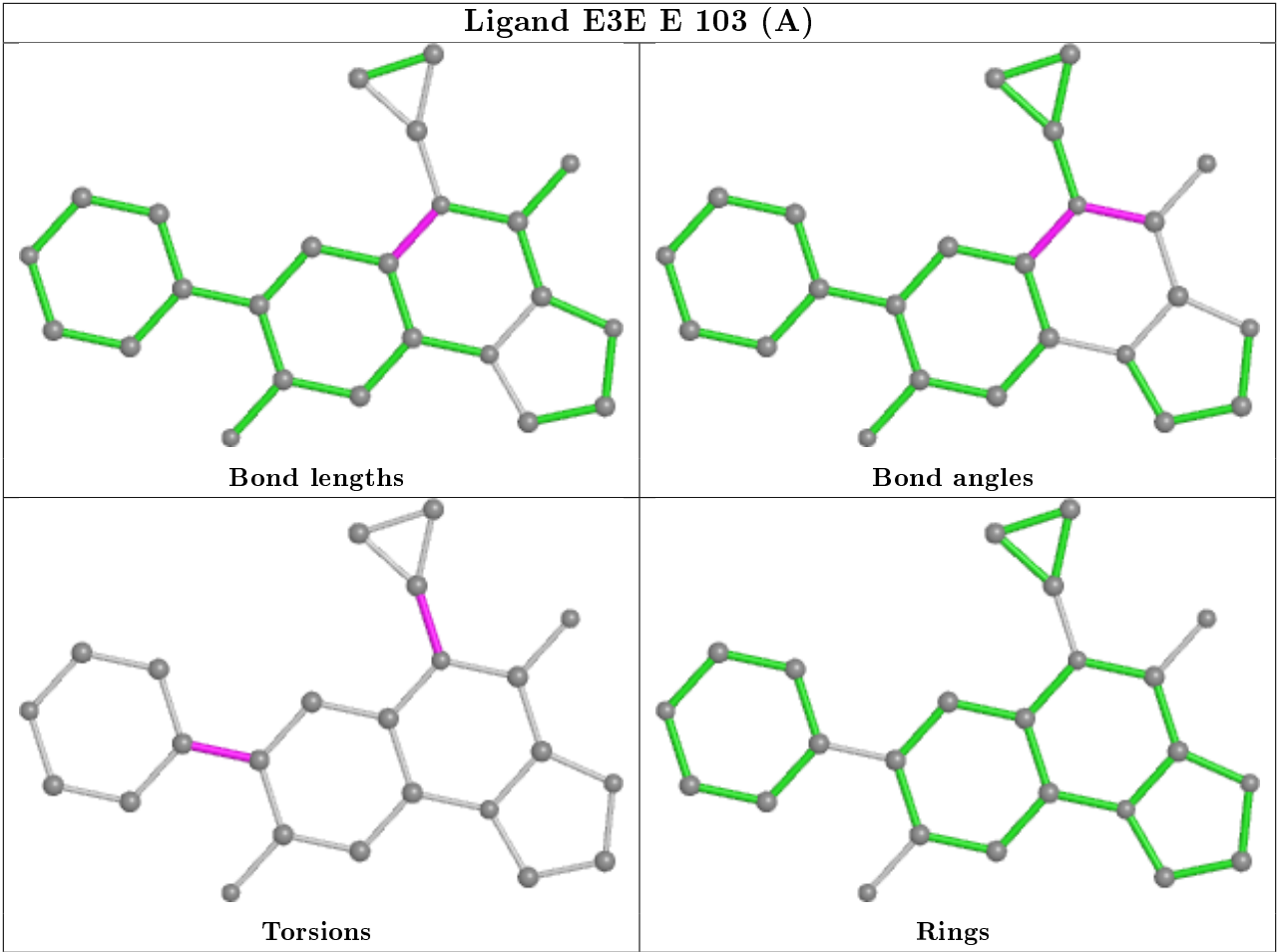
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	502	GOL	2	0
7	E	101	GOL	2	0
9	E	103[A]	E3E	2	0

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.



## Ligand E3E E 102





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	-1[A]:DT	O3'	1[A]:DG	P	5.71

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	189/202 (93%)	1.23	54 (28%) 0 0	63, 112, 198, 218	0
1	D	189/202 (93%)	1.17	50 (26%) 0 0	80, 133, 177, 198	0
2	A	481/490 (98%)	-0.21	0 100 100	45, 72, 107, 168	0
3	C	480/490 (97%)	-0.24	1 (0%) 95 91	43, 69, 102, 175	0
4	E	20/20 (100%)	-0.01	0 100 100	61, 79, 135, 135	0
4	F	20/20 (100%)	0.27	1 (5%) 28 13	61, 78, 141, 158	0
All	All	1379/1424 (96%)	0.17	106 (7%) 13 5	43, 78, 163, 218	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	581	LYS	11.1
1	B	580	TYR	8.7
1	B	582	GLY	8.7
1	B	544	THR	7.3
1	B	423	SER	7.0
1	B	443	THR	6.2
1	B	591	LEU	5.9
1	B	586	MET	5.6
1	B	594	THR	5.3
1	B	440	GLY	5.3
1	D	485	PHE	4.9
1	B	438[A]	SER	4.9
1	B	543	PRO	4.8
1	D	532	ILE	4.8
1	B	437[A]	ASP	4.7
1	B	583	LEU	4.7
1	B	587	ASN	4.6
1	D	524	PHE	4.6
1	B	593	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	523	PHE	4.3
1	D	505	ILE	4.2
1	B	422	SER	4.2
1	B	590	GLN	4.1
1	D	498	ALA	4.0
4	F	12	DT	4.0
1	D	495	LEU	3.9
1	D	588	ALA	3.8
1	B	445	SER	3.8
1	D	489	ILE	3.8
1	D	439	ALA	3.8
1	B	418	LEU	3.8
1	B	421	CYS	3.7
1	D	432	PHE	3.7
1	B	420	ASP	3.7
1	D	521	LEU	3.6
1	D	528	MET	3.5
1	B	589	ASP	3.5
1	D	503	ILE	3.5
1	D	536	TYR	3.4
1	D	587	ASN	3.4
1	B	600	HIS	3.4
1	D	481	MET	3.3
1	B	447	ARG	3.3
1	B	588	ALA	3.3
1	D	545	GLY	3.3
1	B	595	THR	3.1
1	D	581	LYS	3.1
1	B	598	PRO	3.1
1	D	443	THR	3.0
1	D	431	ILE	3.0
1	D	506	MET	3.0
1	D	487	THR	2.9
1	B	596	MET	2.9
3	C	14	ILE	2.9
1	D	490	GLY	2.8
1	B	485	PHE	2.8
1	B	417	LYS	2.8
1	D	504	VAL	2.8
1	D	434	VAL	2.8
1	D	609	GLU	2.8
1	B	454	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	446	GLY	2.7
1	B	487	THR	2.7
1	B	453	ALA	2.7
1	B	592	TRP	2.6
1	D	539	ILE	2.6
1	B	444	LYS	2.6
1	D	502	LYS	2.6
1	D	608	LEU	2.6
1	D	602	ALA	2.6
1	B	531	LEU	2.6
1	D	534	ALA	2.6
1	D	520	LEU	2.6
1	B	419	ALA	2.6
1	D	606	VAL	2.5
1	B	442	SER	2.5
1	B	500	TYR	2.5
1	D	525	TYR	2.5
1	B	599	GLU	2.5
1	D	496	ALA	2.5
1	D	430	GLU	2.5
1	B	439[A]	ALA	2.4
1	B	426	PRO	2.4
1	B	597	ASN	2.4
1	D	436	GLY	2.4
1	B	584	GLY	2.4
1	B	536	TYR	2.4
1	B	448	ASP	2.3
1	D	618	PHE	2.3
1	D	580	TYR	2.3
1	B	498	ALA	2.3
1	D	493	PHE	2.3
1	D	590	GLN	2.2
1	B	432	PHE	2.2
1	D	607	LYS	2.2
1	B	441	GLY	2.2
1	D	445	SER	2.2
1	B	486	GLY	2.2
1	B	452	GLN	2.1
1	D	535	GLY	2.1
1	D	501	HIS	2.1
1	D	461	ILE	2.0
1	B	499	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	453	ALA	2.0
1	D	583	LEU	2.0
1	D	611	ALA	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PTR	C	123	16/17	0.93	0.27	61,89,119,130	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	GOL	C	504	6/6	0.66	0.30	87,102,110,115	0
7	GOL	C	502	6/6	0.72	0.52	107,117,122,141	0
7	GOL	C	503	6/6	0.73	0.60	158,158,163,167	0
7	GOL	A	502	6/6	0.76	0.44	120,135,146,149	0
7	GOL	A	504	6/6	0.78	0.46	101,114,119,121	0
7	GOL	A	503	6/6	0.81	0.25	92,109,114,120	0
7	GOL	A	505	6/6	0.81	0.37	99,104,105,112	0
7	GOL	E	101	6/6	0.86	0.25	95,100,118,118	0
9	E3E	E	103[B]	24/24	0.87	0.33	112,127,170,178	24
9	E3E	E	103[A]	24/24	0.87	0.33	110,124,166,173	24
8	SO4	C	501	5/5	0.89	0.15	140,145,151,160	0
5	MN	B	701	1/1	0.91	0.20	114,114,114,114	0
6	NA	A	501	1/1	0.92	0.09	105,105,105,105	0
5	MN	D	701	1/1	0.93	0.17	153,153,153,153	0

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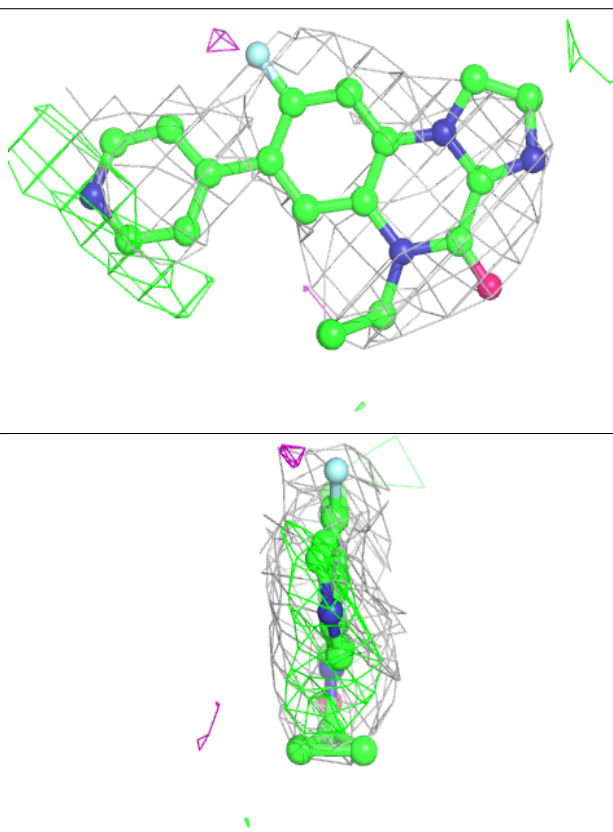
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	E3E	E	102	24/24	0.94	0.18	74,97,108,114	0

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.

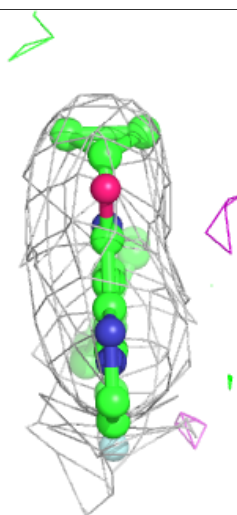
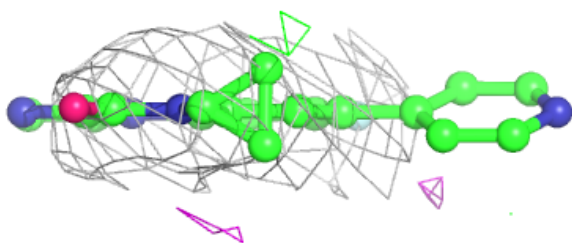
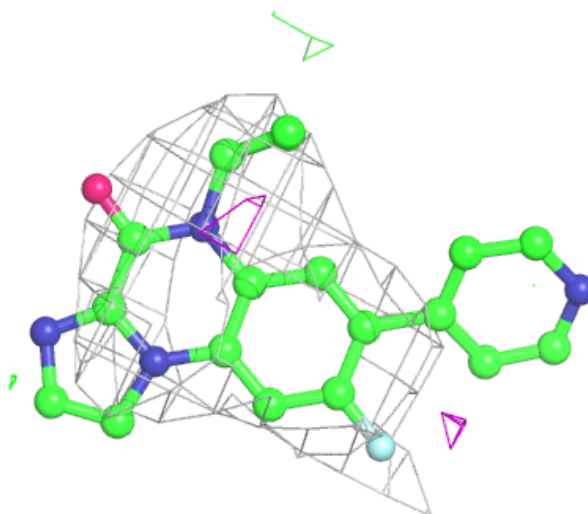
**Electron density around E3E E 103 (B):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



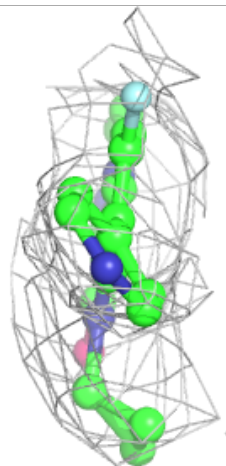
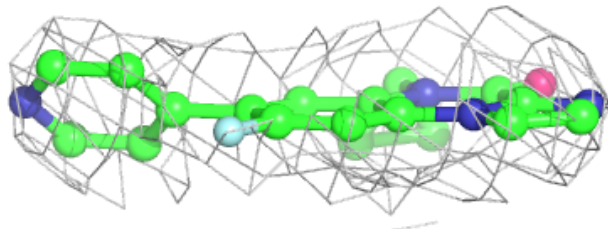
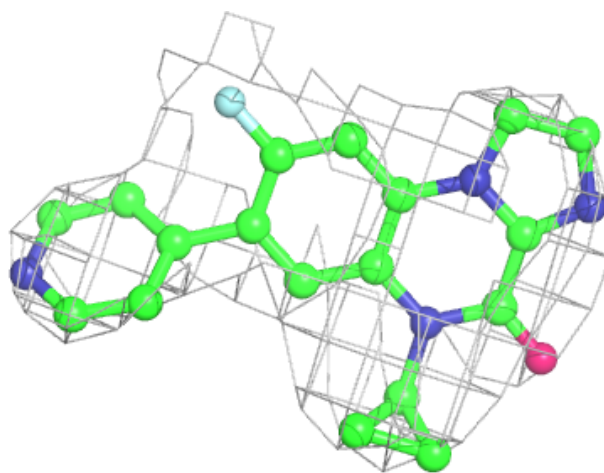
**Electron density around E3E E 103 (A):**

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



**Electron density around E3E E 102:**

$2mF_o-DF_c$  (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.