Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 12:51 pm GMT

PDB ID	:	5IWI
Title	:	1.98A structure of GSK945237 with S.aureus DNA gyrase and singly nicked DNA
Authors	:	Bax, B.D.; Miles, T.J.
Deposited on	:	2016-03-22
Resolution	:	1.98 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

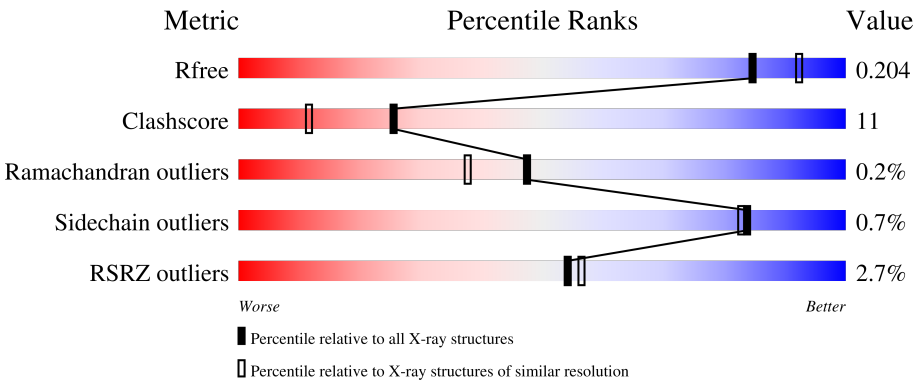
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	202	6% 77% 16% • 5%
1	D	202	6% 79% 14% • 6%
2	A	490	2% 88% 10% •
2	C	490	% 87% 11% •
3	E	20	35% 60% 5%

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Mol	Chain	Length	Quality of chain
4	F	8	100%
5	G	12	8% 83% 8%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14196 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
			Total	C	N	O	S			
1	B	192	1709	1067	293	339	10	0	27	0
1	D	189	1661	1033	291	328	9	0	23	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	expression tag	UNP P66937
B	544	THR	-	linker	UNP P66937
B	545	GLY	-	linker	UNP P66937
D	409	MET	-	expression tag	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
			Total	C	N	O	S			
2	A	483	4034	2497	737	782	18	0	23	0
2	C	481	4091	2531	750	790	20	0	30	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	PHE	TYR	conflict	UNP Q99XG5
C	123	PHE	TYR	conflict	UNP Q99XG5

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*AP*CP*CP*GP*CP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	20	796	377	155	226	38	0	20	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	F	8	328	158	58	98	14	0	8	0

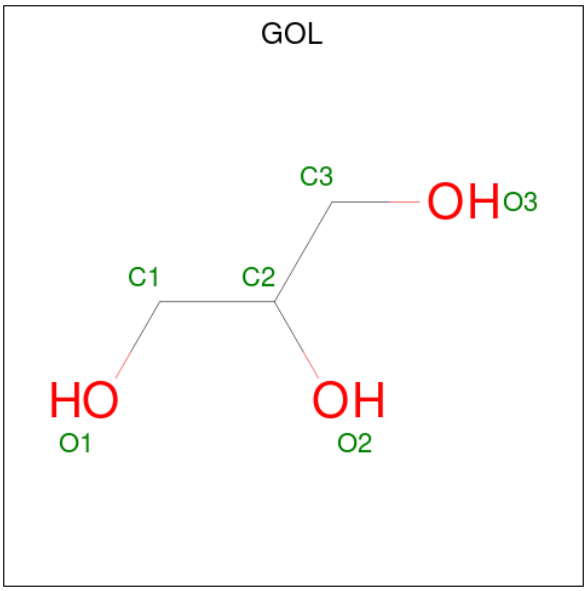
- Molecule 5 is a DNA chain called DNA (5'-D(*TP*GP*TP*GP*CP*GP*GP*T*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	G	12	468	224	84	138	22	0	12	0

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
6	B	1	2	2	0	1
6	D	1	2	2	0	1
6	C	1	1	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



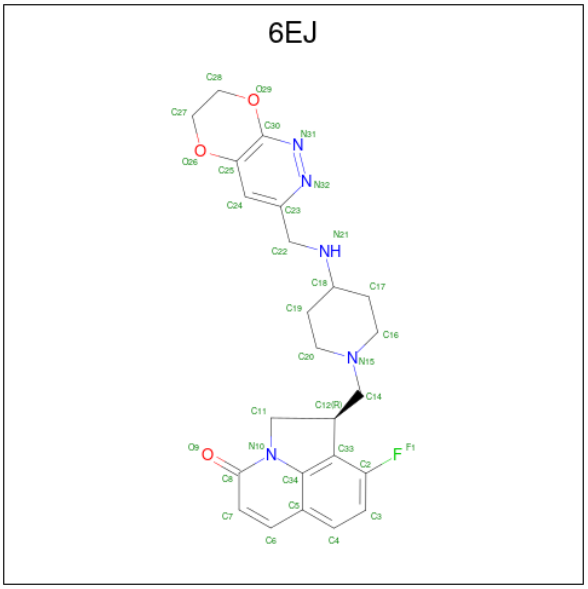
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	6	3	3	0	0
			Total	C	O		
7	A	1	6	3	3	0	0
			Total	C	O		
7	A	1	6	3	3	0	0
			Total	C	O		
7	A	1	6	3	3	0	0
			Total	C	O		
7	A	1	6	3	3	0	0
			Total	C	O		
7	A	1	6	3	3	0	0
			Total	C	O		
7	C	1	6	3	3	0	0
			Total	C	O		
7	C	1	12	6	6	0	1
			Total	C	O		
7	C	1	6	3	3	0	0
			Total	C	O		
7	C	1	6	3	3	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	A	1	1	1	0	0

- Molecule 9 is (1R)-1-[(4-{[(6,7-dihydro[1,4]dioxino[2,3-c]pyridazin-3-yl)methyl]amino}piperi

din-1-yl)methyl]-9-fluoro-1,2-dihydro-4H-pyrrolo[3,2,1-ij]quinolin-4-one (three-letter code: 6EJ) (formula: $C_{24}H_{26}FN_5O_3$).



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

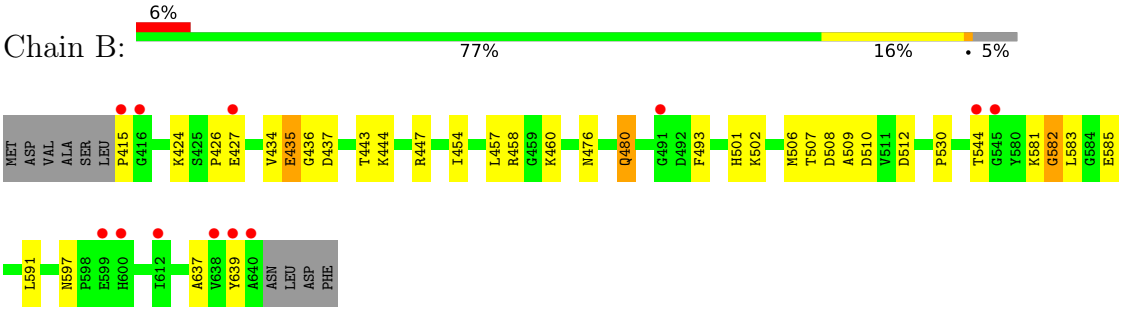
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	B	94	98	98	0	4
10	A	341	345	345	0	4
10	D	56	59	59	0	3
10	C	355	358	358	0	4
10	E	49	52	52	0	3
10	F	21	21	21	0	0
10	G	34	38	38	0	4

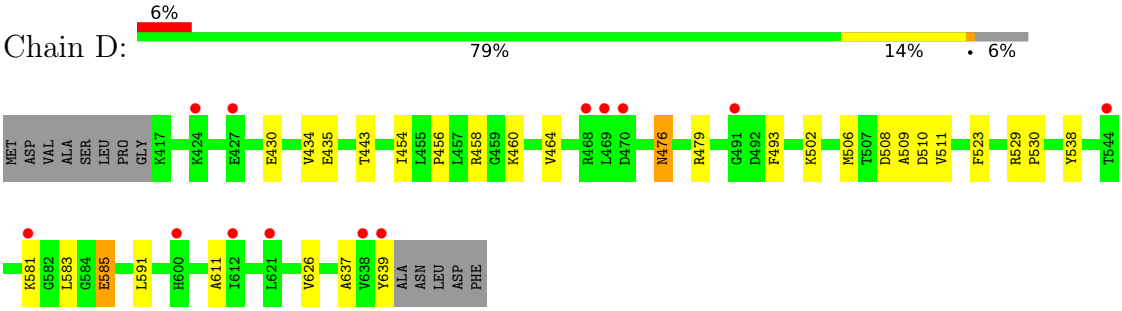
3 Residue-property plots (i)

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.

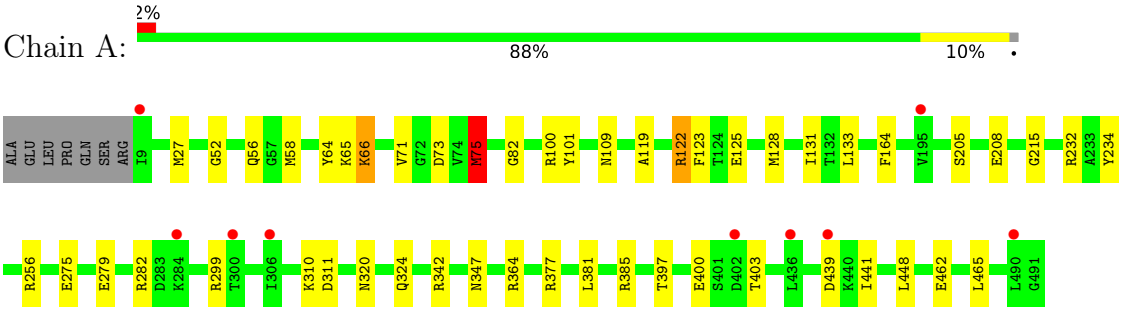
• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B



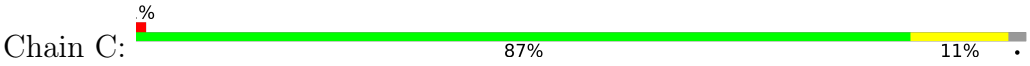
• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B

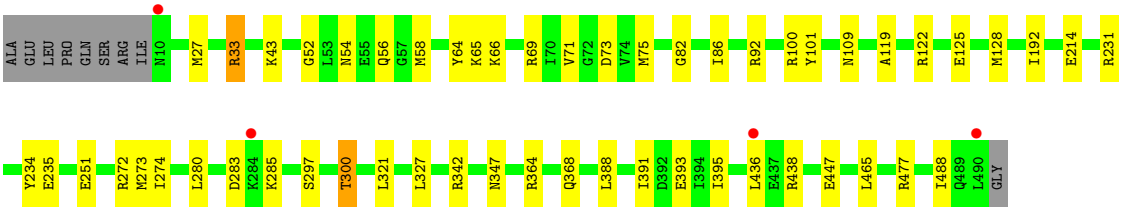


• Molecule 2: DNA gyrase subunit A



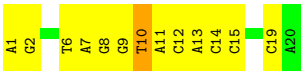
• Molecule 2: DNA gyrase subunit A





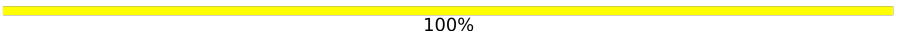
• Molecule 3: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*AP*CP*CP*GP*CP*AP*CP*A)-3')

Chain E:



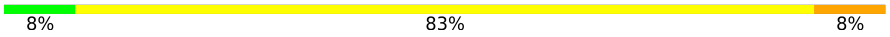
• Molecule 4: DNA (5'-D(*TP*GP*TP*GP*CP*GP*GP*T*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')

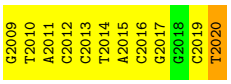
Chain F:



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

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	92.90Å 92.90Å 410.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.00 – 1.98 19.90 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.2 (18.00-1.98) 99.3 (19.90-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.166 , 0.202 0.169 , 0.204	Depositor DCC
R_{free} test set	2761 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14196	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN, 6EJ, CL

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	0.44	0/1735	0.70	0/2339
1	D	0.46	0/1685	0.71	0/2273
2	A	0.47	0/4082	0.69	3/5487 (0.1%)
2	C	0.47	0/4139	0.69	0/5564
3	E	0.36	0/912	0.77	2/1402 (0.1%)
4	F	0.29	0/366	0.70	0/564
5	G	579.66	4/538 (0.7%)	9.58	12/826 (1.5%)
All	All	115.90	4/13457 (0.0%)	2.14	17/18455 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	2020[A]	DT	C4'-C3'	6791.13	69.44	1.53
5	G	2020[B]	DT	C4'-C3'	6791.13	69.44	1.53
5	G	2020[A]	DT	C4'-O4'	6653.22	67.98	1.45
5	G	2020[B]	DT	C4'-O4'	6653.22	67.98	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	2020[A]	DT	O4'-C4'-C3'	-174.12	1.53	106.00
5	G	2020[B]	DT	O4'-C4'-C3'	-174.12	1.53	106.00
5	G	2020[A]	DT	C4'-C3'-C2'	-71.22	39.00	103.10
5	G	2020[B]	DT	C4'-C3'-C2'	-71.22	39.00	103.10
5	G	2020[A]	DT	C1'-O4'-C4'	-44.23	65.86	110.10
5	G	2020[B]	DT	C1'-O4'-C4'	-44.23	65.86	110.10
5	G	2020[A]	DT	C5'-C4'-C3'	-12.26	92.04	114.10
5	G	2020[B]	DT	C5'-C4'-C3'	-12.26	92.04	114.10
5	G	2020[A]	DT	C5'-C4'-O4'	-9.81	90.67	109.30
5	G	2020[B]	DT	C5'-C4'-O4'	-9.81	90.67	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	122[A]	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	A	122[B]	ARG	NE-CZ-NH2	-6.08	117.26	120.30
3	E	10[A]	DT	C1'-O4'-C4'	-5.75	104.35	110.10
3	E	10[B]	DT	C1'-O4'-C4'	-5.75	104.35	110.10
2	A	75	MET	CG-SD-CE	-5.56	91.30	100.20
5	G	2016[A]	DC	C1'-O4'-C4'	-5.07	105.03	110.10
5	G	2016[B]	DC	C1'-O4'-C4'	-5.07	105.03	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1709	0	1660	54	0
1	D	1661	0	1610	50	0
2	A	4034	0	4047	62	0
2	C	4091	0	4115	64	0
3	E	796	0	397	38	0
4	F	328	0	168	17	0
5	G	468	0	236	38	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	36	0	48	0	0
7	C	30	0	40	1	0
8	A	1	0	0	0	0
9	E	66	0	0	1	0
10	A	345	0	0	10	0
10	B	98	0	0	3	0
10	C	358	0	0	8	0
10	D	59	0	0	8	0
10	E	52	0	0	1	0
10	F	21	0	0	3	0
10	G	38	0	0	1	0
All	All	14196	0	12321	269	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 11.

All (269) 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)
2:A:27[B]:MET:HA	2:A:27[B]:MET:CE	1.57	1.33
5:G:2009[B]:DG:C3'	5:G:2010[B]:DT:H71	1.60	1.29
5:G:2009[B]:DG:H3'	5:G:2010[B]:DT:C7	1.61	1.27
10:D:1150[B]:HOH:O	3:E:10[B]:DT:C5'	1.83	1.24
10:D:1150[B]:HOH:O	3:E:10[B]:DT:H5'	1.40	1.11
2:A:27[B]:MET:HA	2:A:27[B]:MET:HE3	1.11	1.08
1:B:585[B]:GLU:OE1	1:B:585[B]:GLU:O	1.69	1.06
1:B:435[A]:GLU:O	1:B:457[A]:LEU:O	1.70	1.06
5:G:2009[B]:DG:C5	5:G:2010[B]:DT:O4	2.11	1.02
5:G:2009[B]:DG:H2'	5:G:2010[B]:DT:C5	1.95	1.01
2:A:66[B]:LYS:HE2	1:D:581[B]:LYS:NZ	1.74	1.01
2:A:66[B]:LYS:HE2	1:D:581[B]:LYS:HZ3	1.23	0.98
2:A:27[B]:MET:HE3	2:A:27[B]:MET:CA	1.94	0.97
2:A:58[B]:MET:HE3	10:A:783:HOH:O	1.64	0.97
2:A:66[A]:LYS:H	2:A:66[A]:LYS:CE	1.80	0.94
1:D:510[B]:ASP:OD2	10:D:1101:HOH:O	1.85	0.93
1:B:508[B]:ASP:CG	1:B:582[B]:GLY:HA2	1.89	0.92
1:B:508[B]:ASP:OD2	1:B:582[B]:GLY:HA2	1.72	0.90
2:A:66[B]:LYS:CE	1:D:581[B]:LYS:NZ	2.33	0.90
1:D:458[B]:ARG:HH12	3:E:11[B]:DA:C5'	1.84	0.90
3:E:2[B]:DG:O6	5:G:2019[B]:DC:N4	2.05	0.90
2:A:27[B]:MET:CE	2:A:27[B]:MET:CA	2.45	0.89
1:B:508[B]:ASP:OD1	1:B:582[B]:GLY:HA2	1.73	0.88
2:A:27[B]:MET:HA	2:A:27[B]:MET:HE2	1.52	0.88
1:D:508[B]:ASP:OD2	1:D:581[B]:LYS:O	1.92	0.88
1:B:581[B]:LYS:HE2	2:C:66[B]:LYS:NZ	1.88	0.88
2:A:66[A]:LYS:H	2:A:66[A]:LYS:HE2	1.39	0.87
5:G:2009[B]:DG:H3'	5:G:2010[B]:DT:H71	0.88	0.87
2:C:58[B]:MET:CE	2:C:65[B]:LYS:HB2	2.05	0.87
2:C:58[B]:MET:HE1	2:C:65[B]:LYS:HB2	1.57	0.85
1:B:639[B]:TYR:CE1	2:A:27[B]:MET:SD	2.70	0.84
5:G:2009[B]:DG:C4	5:G:2010[B]:DT:O4	2.30	0.84
5:G:2010[B]:DT:H6	5:G:2010[B]:DT:O5'	1.60	0.83
1:B:437[B]:ASP:OD1	1:B:458[B]:ARG:NH1	2.12	0.82
1:D:458[B]:ARG:HG3	3:E:9[B]:DG:H2"	1.61	0.82
1:D:458[B]:ARG:HH12	3:E:11[B]:DA:H5'	1.42	0.81
2:C:214[A]:GLU:HG2	2:C:488:ILE:HD12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:128:MET:HE1	2:A:133:LEU:HD23	1.63	0.81
1:B:476:ASN:O	1:B:480:GLN:HG2	1.79	0.81
2:A:66[B]:LYS:CE	1:D:581[B]:LYS:HZ3	1.93	0.81
5:G:2009[B]:DG:C4	5:G:2010[B]:DT:C4	2.70	0.79
1:B:415:PRO:HB3	1:B:480:GLN:NE2	1.97	0.79
5:G:2009[B]:DG:C3'	5:G:2010[B]:DT:C7	2.38	0.78
3:E:2[B]:DG:N1	5:G:2019[B]:DC:N3	2.32	0.78
1:B:443[B]:THR:HG22	1:B:591:LEU:HD21	1.67	0.77
1:D:458[B]:ARG:HD2	3:E:10[B]:DT:C1'	2.16	0.76
5:G:2009[B]:DG:H2'	5:G:2010[B]:DT:C6	2.20	0.75
2:A:66[A]:LYS:H	2:A:66[A]:LYS:CD	2.00	0.75
3:E:19[B]:DC:N3	4:F:1002[B]:DG:N1	2.30	0.75
2:C:273[B]:MET:HG3	2:C:274:ILE:N	2.00	0.74
1:B:447:ARG:HD3	1:B:454:ILE:HD11	1.70	0.73
1:D:458[B]:ARG:NH1	3:E:11[B]:DA:H5'	2.03	0.73
1:B:508[B]:ASP:OD2	1:B:582[B]:GLY:CA	2.37	0.72
2:C:73[A]:ASP:OD1	10:C:601:HOH:O	2.07	0.72
2:C:66[A]:LYS:HD3	2:C:66[A]:LYS:N	2.06	0.71
3:E:1[B]:DA:N7	5:G:2020[B]:DT:N3	2.38	0.71
2:C:58[B]:MET:CE	2:C:65[B]:LYS:CB	2.69	0.71
2:C:66[A]:LYS:H	2:C:66[A]:LYS:CE	2.04	0.70
2:A:66[B]:LYS:CE	1:D:581[B]:LYS:HZ1	2.01	0.70
1:B:639[B]:TYR:HE1	2:A:27[B]:MET:CE	2.05	0.70
2:A:73[A]:ASP:OD1	10:C:601:HOH:O	2.10	0.69
1:D:458[B]:ARG:HD2	3:E:10[B]:DT:H1'	1.75	0.69
1:B:510[A]:ASP:OD2	10:B:802:HOH:O	2.10	0.69
5:G:2009[B]:DG:C2'	5:G:2010[B]:DT:C7	2.71	0.69
1:B:581[B]:LYS:HE2	2:C:66[B]:LYS:HZ1	1.56	0.68
2:A:66[A]:LYS:HB3	10:A:737[A]:HOH:O	1.94	0.68
2:A:66[A]:LYS:HD3	2:A:66[A]:LYS:N	2.09	0.68
1:D:443[A]:THR:CG2	1:D:454:ILE:HD12	2.23	0.68
2:C:71:VAL:O	2:C:75:MET:HG3	1.94	0.67
1:B:581[B]:LYS:CE	2:C:66[B]:LYS:NZ	2.58	0.67
1:D:443[A]:THR:HG22	1:D:454:ILE:HD12	1.77	0.67
2:A:66[A]:LYS:CD	2:A:66[A]:LYS:N	2.58	0.67
2:C:231[B]:ARG:O	2:C:235[B]:GLU:HG3	1.95	0.67
2:C:66[A]:LYS:H	2:C:66[A]:LYS:CD	2.08	0.66
2:A:123:PHE:O	1:D:585[A]:GLU:HG2	1.96	0.66
2:C:388:LEU:HD13	2:C:438:ARG:HG2	1.77	0.66
5:G:2009[B]:DG:C6	5:G:2010[B]:DT:O4	2.49	0.65
10:D:1150[B]:HOH:O	3:E:10[B]:DT:H5"	1.73	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LYS:HE3	10:B:813:HOH:O	1.96	0.65
1:B:435[B]:GLU:OE1	1:B:508[B]:ASP:N	2.26	0.65
2:A:73[A]:ASP:HA	2:C:69:ARG:HD2	1.79	0.65
1:D:443[A]:THR:HG22	1:D:454:ILE:CD1	2.27	0.64
1:D:435[A]:GLU:HB2	10:D:1102:HOH:O	1.98	0.64
3:E:13[A]:DA:H2'	3:E:14[A]:DC:C6	2.33	0.64
1:B:509[B]:ALA:HB1	1:B:544:THR:HG22	1.80	0.63
3:E:1[B]:DA:N6	5:G:2020[B]:DT:O4	2.32	0.63
5:G:2009[B]:DG:C2'	5:G:2010[B]:DT:H71	2.29	0.63
1:D:581[B]:LYS:HB2	1:D:585[B]:GLU:OE2	1.98	0.63
1:B:639[B]:TYR:HE1	2:A:27[B]:MET:HE2	1.64	0.63
2:A:128:MET:CE	2:A:133:LEU:HD23	2.28	0.62
4:F:1002[B]:DG:H2"	4:F:1003[B]:DT:H72	1.81	0.62
2:C:66[A]:LYS:N	2:C:66[A]:LYS:CD	2.63	0.62
5:G:2009[B]:DG:H2'	5:G:2010[B]:DT:C7	2.29	0.62
5:G:2013[B]:DC:H5"	5:G:2013[B]:DC:H6	1.65	0.62
2:A:66[A]:LYS:HE2	2:A:66[A]:LYS:N	2.14	0.62
1:B:435[B]:GLU:CG	1:B:507[B]:THR:HG22	2.31	0.61
1:D:476[A]:ASN:HA	1:D:479[A]:ARG:HE	1.65	0.60
1:D:443[B]:THR:HG22	1:D:591:LEU:HD21	1.83	0.60
1:B:639[B]:TYR:CE1	2:A:27[B]:MET:CE	2.85	0.60
4:F:1008[B]:DT:O4	10:F:1101:HOH:O	2.16	0.60
1:B:581[B]:LYS:O	1:B:581[B]:LYS:HG3	2.00	0.60
2:A:73[B]:ASP:HA	2:C:69:ARG:HD2	1.83	0.60
3:E:15[A]:DC:H5	10:G:2115:HOH:O	1.84	0.60
3:E:6[B]:DT:H2"	3:E:7[B]:DA:H5"	1.84	0.60
5:G:2009[B]:DG:H8	5:G:2009[B]:DG:HO5'	1.50	0.59
2:C:66[A]:LYS:HD3	2:C:66[A]:LYS:H	1.66	0.59
2:C:273[B]:MET:CE	2:C:327[B]:LEU:HD23	2.32	0.59
2:C:368:GLN:NE2	10:C:604:HOH:O	2.36	0.59
2:A:275[B]:GLU:O	2:A:279[B]:GLU:HG3	2.02	0.58
1:D:458[B]:ARG:HH12	3:E:11[B]:DA:H5"	1.68	0.58
1:D:458[B]:ARG:HD2	3:E:10[B]:DT:O4'	2.03	0.58
2:C:75:MET:HG2	2:C:86:ILE:HD12	1.85	0.58
2:C:297:SER:OG	2:C:300:THR:HG23	2.03	0.58
1:B:424:LYS:O	1:B:426:PRO:HD3	2.03	0.58
2:C:283:ASP:HB2	2:C:285:LYS:HE2	1.86	0.57
1:B:427[B]:GLU:HG2	1:B:501:HIS:CE1	2.39	0.57
5:G:2014[B]:DT:C2'	5:G:2015[B]:DA:O5'	2.53	0.57
1:B:443[B]:THR:CG2	1:B:591:LEU:HD21	2.36	0.56
2:A:71:VAL:O	2:A:75:MET:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458[B]:ARG:NH1	3:E:11[B]:DA:C5'	2.62	0.56
5:G:2009[B]:DG:H3'	5:G:2010[B]:DT:H73	1.76	0.56
1:B:444[A]:LYS:HA	1:B:454:ILE:CD1	2.36	0.55
3:E:14[B]:DC:H2"	3:E:15[B]:DC:H5'	1.87	0.55
1:B:460:LYS:HG3	4:F:1007[B]:DG:H21	1.72	0.55
2:C:58[B]:MET:HE2	2:C:65[B]:LYS:HB3	1.88	0.55
5:G:2010[B]:DT:H71	5:G:2010[B]:DT:OP2	2.06	0.55
2:C:73[A]:ASP:CG	10:C:601:HOH:O	2.43	0.54
3:E:11[B]:DA:H2"	3:E:12[B]:DC:H5"	1.89	0.54
5:G:2010[B]:DT:H71	5:G:2010[B]:DT:P	2.48	0.54
1:B:447:ARG:HD3	1:B:454:ILE:CD1	2.35	0.54
2:C:321:LEU:HB3	2:C:327[B]:LEU:HD12	1.90	0.54
2:A:58[B]:MET:SD	2:A:65[B]:LYS:HD2	2.48	0.54
2:A:256:ARG:HD2	10:A:711:HOH:O	2.07	0.54
2:C:58[B]:MET:HE1	2:C:65[B]:LYS:CB	2.32	0.54
4:F:1006[B]:DG:H2"	4:F:1007[B]:DG:O5'	2.08	0.54
1:B:639[B]:TYR:HE1	2:A:27[B]:MET:SD	2.25	0.54
1:D:626:VAL:HG11	5:G:2017[B]:DG:H3'	1.90	0.53
1:B:415:PRO:HB3	1:B:480:GLN:HE21	1.73	0.53
2:C:43:LYS:NZ	3:E:6[B]:DT:OP1	2.34	0.53
2:A:122[A]:ARG:HD2	2:C:82:GLY:HA2	1.91	0.53
2:A:364:ARG:HB2	2:A:465:LEU:HD11	1.90	0.53
2:C:75:MET:HG2	2:C:86:ILE:CD1	2.39	0.53
1:D:529:ARG:NH2	1:D:611:ALA:HB1	2.24	0.53
4:F:1003[B]:DT:H2"	4:F:1004[B]:DG:C8	2.44	0.53
1:B:581[B]:LYS:CE	2:C:66[B]:LYS:HZ2	2.21	0.53
1:B:435[B]:GLU:HG3	1:B:507[B]:THR:HG22	1.89	0.52
3:E:19[B]:DC:O2	4:F:1002[B]:DG:N2	2.28	0.52
2:A:279[B]:GLU:HG2	2:A:282:ARG:HH12	1.74	0.52
2:C:64:TYR:HB3	2:C:125:GLU:HB3	1.92	0.51
5:G:2010[B]:DT:O5'	5:G:2010[B]:DT:C6	2.52	0.51
2:A:109:ASN:HB3	2:A:119:ALA:HB2	1.92	0.51
3:E:6[B]:DT:C7	10:F:1111:HOH:O	0.82	0.51
5:G:2009[B]:DG:C8	5:G:2010[B]:DT:H73	2.44	0.51
3:E:12[B]:DC:H2"	3:E:13[B]:DA:H5"	1.92	0.51
2:A:397:THR:O	2:A:400[A]:GLU:HG2	2.10	0.51
5:G:2010[B]:DT:H2"	5:G:2011[B]:DA:O5'	2.11	0.51
5:G:2012[A]:DC:H2"	5:G:2013[A]:DC:O5'	2.10	0.51
1:B:444[B]:LYS:HA	1:B:454:ILE:CD1	2.40	0.51
1:D:583[A]:LEU:HD12	10:D:1102:HOH:O	2.10	0.51
2:A:66[B]:LYS:HE3	1:D:581[B]:LYS:HZ1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435[B]:GLU:HG2	1:B:507[B]:THR:HG22	1.92	0.51
2:C:100:ARG:HG3	2:C:101:TYR:CE2	2.45	0.51
2:C:58[B]:MET:HE3	10:C:810:HOH:O	2.11	0.50
5:G:2013[B]:DC:H6	5:G:2013[B]:DC:C5'	2.23	0.50
2:C:235[B]:GLU:CD	10:C:913[B]:HOH:O	2.50	0.50
5:G:2009[B]:DG:C2'	5:G:2010[B]:DT:C5	2.80	0.49
5:G:2009[B]:DG:N3	5:G:2010[B]:DT:C4	2.80	0.49
1:B:457[B]:LEU:O	1:B:458[B]:ARG:HG2	2.13	0.49
1:D:430:GLU:HG2	1:D:502:LYS:HB2	1.95	0.49
1:B:437[B]:ASP:OD1	1:B:437[B]:ASP:N	2.46	0.49
1:D:637:ALA:HB1	2:C:27[A]:MET:HE1	1.94	0.49
1:B:585[B]:GLU:OE1	1:B:585[B]:GLU:C	2.46	0.48
1:D:506:MET:HG2	1:D:583[B]:LEU:HD11	1.95	0.48
1:D:508[B]:ASP:OD1	1:D:509[B]:ALA:N	2.46	0.48
2:C:447:GLU:HG3	10:C:811:HOH:O	2.12	0.48
4:F:1002[B]:DG:H2"	4:F:1003[B]:DT:C7	2.44	0.48
1:D:458[B]:ARG:HG3	3:E:9[B]:DG:C2'	2.38	0.48
2:C:251:GLU:HB3	7:C:503[A]:GOL:H32	1.95	0.48
2:A:100:ARG:HG3	2:A:101:TYR:CE2	2.48	0.48
1:B:493:PHE:CE2	1:B:530:PRO:HB2	2.49	0.48
5:G:2014[B]:DT:H2'	5:G:2015[B]:DA:O5'	2.14	0.48
3:E:7[B]:DA:H2'	3:E:8[B]:DG:C8	2.49	0.47
2:C:65[B]:LYS:HE2	2:C:69:ARG:HG2	1.95	0.47
3:E:14[B]:DC:C2'	3:E:15[B]:DC:H5'	2.45	0.47
10:D:1150[B]:HOH:O	3:E:10[B]:DT:H4'	2.12	0.47
3:E:6[B]:DT:H71	10:F:1111:HOH:O	0.76	0.47
1:D:443[B]:THR:CG2	1:D:591:LEU:HD21	2.44	0.47
5:G:2009[B]:DG:C2	5:G:2010[B]:DT:N3	2.82	0.47
1:D:464:VAL:HG21	1:D:523:PHE:HA	1.97	0.46
1:B:508[B]:ASP:OD2	1:B:582[B]:GLY:N	2.48	0.46
5:G:2012[B]:DC:C2	5:G:2013[B]:DC:C5	3.03	0.46
1:B:639[B]:TYR:CD2	2:A:342:ARG:HG2	2.50	0.46
2:C:58[B]:MET:HE2	2:C:65[B]:LYS:CB	2.40	0.46
2:C:393[B]:GLU:HG2	10:C:889[B]:HOH:O	2.16	0.46
3:E:13[B]:DA:H2'	3:E:14[B]:DC:C6	2.51	0.46
1:B:508[B]:ASP:CG	1:B:582[B]:GLY:CA	2.74	0.45
1:B:443[A]:THR:HG22	1:B:454:ILE:HG12	1.98	0.45
2:A:64:TYR:HB3	2:A:125:GLU:HB3	1.97	0.45
1:D:434[B]:VAL:HG23	1:D:456:PRO:HA	1.98	0.45
2:A:122[A]:ARG:HG3	10:A:807:HOH:O	2.16	0.45
2:C:280:LEU:HD23	2:C:285:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458[B]:ARG:NH1	3:E:10[B]:DT:O3'	2.49	0.45
2:C:273[B]:MET:HE1	2:C:327[B]:LEU:HD23	1.98	0.45
1:B:581[B]:LYS:O	1:B:582[B]:GLY:O	2.35	0.45
2:A:27[B]:MET:CA	2:A:27[B]:MET:HE2	2.34	0.45
2:A:381:LEU:HD22	2:A:441:ILE:HG23	1.98	0.45
1:D:511[B]:VAL:HG13	10:D:1149:HOH:O	2.16	0.45
1:B:444[A]:LYS:HA	1:B:454:ILE:HD13	1.99	0.45
2:A:205:SER:OG	2:A:208:GLU:HG3	2.16	0.44
2:C:391:ILE:O	2:C:395:ILE:HG12	2.16	0.44
2:C:33:ARG:CZ	4:F:1007[A]:DG:H4'	2.47	0.44
1:B:427[B]:GLU:HG3	10:B:878:HOH:O	2.17	0.44
4:F:1001[A]:DT:H2"	4:F:1002[A]:DG:C8	2.52	0.44
5:G:2013[B]:DC:C5'	5:G:2013[B]:DC:C6	3.00	0.44
1:D:476[A]:ASN:CB	1:D:479[A]:ARG:HH21	2.29	0.44
2:C:234:TYR:O	2:C:347:ASN:HB2	2.18	0.44
2:C:54:ASN:HA	2:C:128:MET:CE	2.48	0.44
1:D:493:PHE:CE1	1:D:530:PRO:HB2	2.53	0.43
2:A:52:GLY:O	2:A:56[B]:GLN:HG3	2.18	0.43
1:D:443[A]:THR:HG21	1:D:454:ILE:HD12	1.97	0.43
1:D:458[B]:ARG:HD3	3:E:10[B]:DT:H4'	1.99	0.43
2:C:109:ASN:HB3	2:C:119:ALA:HB2	2.00	0.43
2:A:462:GLU:HG2	10:A:694:HOH:O	2.17	0.43
3:E:6[A]:DT:H2"	3:E:7[A]:DA:H5"	2.01	0.43
2:A:310:LYS:O	2:A:311:ASP:HB2	2.18	0.43
5:G:2010[B]:DT:C7	5:G:2010[B]:DT:OP2	2.66	0.43
1:B:435[A]:GLU:C	1:B:457[A]:LEU:O	2.50	0.43
2:A:215:GLY:HA2	2:A:234:TYR:OH	2.18	0.43
1:B:506:MET:HG2	1:B:583[A]:LEU:HD11	2.01	0.43
1:D:502:LYS:HG2	1:D:538:TYR:CE1	2.53	0.43
2:A:377:ARG:HG3	2:A:448:LEU:HD11	2.00	0.42
1:D:508[B]:ASP:CG	1:D:581[B]:LYS:O	2.54	0.42
2:A:232[B]:ARG:HD2	10:A:620:HOH:O	2.18	0.42
2:A:66[A]:LYS:HE3	10:A:605:HOH:O	2.20	0.42
2:A:82:GLY:HA2	2:C:122[B]:ARG:HD2	2.01	0.42
2:A:320:ASN:HB3	2:A:324:GLN:HE21	1.85	0.42
3:E:9[A]:DG:H5"	3:E:9[A]:DG:H8	1.83	0.42
1:D:639:TYR:CG	2:C:342[B]:ARG:HG2	2.54	0.42
2:C:92:ARG:NH2	4:F:1006[A]:DG:OP2	2.46	0.42
3:E:10[A]:DT:C2	9:E:101[A]:6EJ:C8	3.03	0.42
2:C:272[A]:ARG:CZ	4:F:1003[A]:DT:H5"	2.49	0.42
2:C:364:ARG:HB2	2:C:465:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:385:ARG:NH1	10:A:609:HOH:O	2.52	0.42
2:C:52:GLY:O	2:C:56[B]:GLN:HG3	2.19	0.41
2:C:66[A]:LYS:H	2:C:66[A]:LYS:HE2	1.80	0.41
10:A:613:HOH:O	4:F:1008[B]:DT:C7	2.68	0.41
5:G:2019[B]:DC:C6	5:G:2020[B]:DT:H72	2.55	0.41
1:B:512:ASP:HB3	4:F:1008[B]:DT:H4'	2.03	0.41
2:A:234:TYR:O	2:A:347:ASN:HB2	2.19	0.41
2:C:66[A]:LYS:HE2	2:C:66[A]:LYS:HB2	1.76	0.41
2:C:214[A]:GLU:HG2	2:C:488:ILE:CD1	2.42	0.41
2:A:439:ASP:HB2	10:A:616:HOH:O	2.20	0.41
1:D:476[A]:ASN:CA	1:D:479[A]:ARG:HH21	2.33	0.41
1:D:476[A]:ASN:HA	1:D:479[A]:ARG:HH21	1.85	0.41
2:A:75:MET:CE	2:C:122[B]:ARG:HB3	2.50	0.41
2:A:403:THR:HG22	2:C:436:LEU:HD22	2.01	0.41
1:D:434[B]:VAL:HG11	1:D:443[B]:THR:HG21	2.02	0.41
2:C:122[A]:ARG:NH2	3:E:9[A]:DG:H5'	2.36	0.41
2:C:272[A]:ARG:NH2	4:F:1003[A]:DT:OP1	2.54	0.41
1:B:434[B]:VAL:O	1:B:436[B]:GLY:N	2.54	0.41
1:B:581[B]:LYS:C	1:B:582[B]:GLY:O	2.58	0.41
1:D:460:LYS:HG3	4:F:1007[A]:DG:H21	1.86	0.41
2:C:58[B]:MET:SD	2:C:65[B]:LYS:HD2	2.61	0.41
10:E:233:HOH:O	4:F:1005[B]:DC:H5	2.04	0.41
1:B:444[A]:LYS:O	1:B:447:ARG:HG2	2.21	0.40
1:B:637:ALA:HB1	2:A:27[B]:MET:SD	2.61	0.40
2:A:131:ILE:HG12	2:A:164:PHE:CE1	2.56	0.40
1:D:508[A]:ASP:OD1	1:D:583[A]:LEU:HG	2.22	0.40
2:C:192:ILE:HG21	2:C:477:ARG:HB2	2.03	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	217/202 (107%)	200 (92%)	13 (6%)	4 (2%)	8	1
1	D	210/202 (104%)	202 (96%)	8 (4%)	0	100	100
2	A	504/490 (103%)	493 (98%)	11 (2%)	0	100	100
2	C	509/490 (104%)	500 (98%)	8 (2%)	1 (0%)	47	38
All	All	1440/1384 (104%)	1395 (97%)	40 (3%)	5 (0%)	47	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	435[A]	GLU
1	B	435[B]	GLU
1	B	582[A]	GLY
1	B	582[B]	GLY
2	C	33	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	180/168 (107%)	178 (99%)	2 (1%)	73	70
1	D	175/168 (104%)	171 (98%)	4 (2%)	50	44
2	A	437/423 (103%)	433 (99%)	4 (1%)	78	77
2	C	446/423 (105%)	445 (100%)	1 (0%)	93	93
All	All	1238/1182 (105%)	1227 (99%)	11 (1%)	84	77

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	480	GLN
1	B	597	ASN
2	A	66[A]	LYS
2	A	66[B]	LYS
2	A	75	MET
2	A	299	ARG

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Mol	Chain	Res	Type
1	D	476[A]	ASN
1	D	476[B]	ASN
1	D	585[A]	GLU
1	D	585[B]	GLU
2	C	300	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	480	GLN
1	B	501	HIS
1	B	597	ASN
2	A	324	GLN
2	A	368	GLN
2	A	390	HIS
2	C	334	ASN
2	C	368	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
7	GOL	C	503[A]	-	5,5,5	0.26	0	5,5,5	0.34	0
9	6EJ	E	101[B]	-	36,38,38	0.89	0	40,55,55	1.32	8 (20%)
7	GOL	A	506	-	5,5,5	0.30	0	5,5,5	0.42	0
7	GOL	C	505	-	5,5,5	0.31	0	5,5,5	0.87	0
7	GOL	A	505	-	5,5,5	0.35	0	5,5,5	0.42	0
7	GOL	C	503[B]	-	5,5,5	0.24	0	5,5,5	0.33	0
7	GOL	C	504	-	5,5,5	0.43	0	5,5,5	0.37	0
7	GOL	A	504	-	5,5,5	0.33	0	5,5,5	0.33	0
7	GOL	C	502	-	5,5,5	0.32	0	5,5,5	0.39	0
9	6EJ	E	101[A]	-	36,38,38	0.93	1 (2%)	40,55,55	1.12	3 (7%)
7	GOL	A	502	-	5,5,5	0.25	0	5,5,5	0.65	0
7	GOL	A	501	-	5,5,5	0.33	0	5,5,5	0.69	0
7	GOL	A	503	-	5,5,5	0.19	0	5,5,5	0.39	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
7	GOL	C	503[A]	-	-	4/4/4/4	-
9	6EJ	E	101[B]	-	-	5/9/34/34	0/6/6/6
7	GOL	A	506	-	-	0/4/4/4	-
7	GOL	C	505	-	-	3/4/4/4	-
7	GOL	A	505	-	-	4/4/4/4	-
7	GOL	C	503[B]	-	-	2/4/4/4	-
7	GOL	C	504	-	-	2/4/4/4	-
7	GOL	A	504	-	-	0/4/4/4	-
7	GOL	C	502	-	-	2/4/4/4	-
9	6EJ	E	101[A]	-	-	2/9/34/34	0/6/6/6
7	GOL	A	502	-	-	2/4/4/4	-
7	GOL	A	501	-	-	3/4/4/4	-
7	GOL	A	503	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	101[A]	6EJ	C30-N31	2.47	1.34	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	101[B]	6EJ	O9-C8-N10	2.77	125.71	120.31
9	E	101[A]	6EJ	O9-C8-N10	2.36	124.91	120.31
9	E	101[B]	6EJ	O26-C25-C30	2.34	123.51	121.83
9	E	101[B]	6EJ	C14-C12-C33	-2.33	106.43	111.65
9	E	101[B]	6EJ	C5-C34-N10	2.23	124.48	123.31
9	E	101[B]	6EJ	C34-N10-C8	-2.21	121.58	123.42
9	E	101[B]	6EJ	C4-C5-C6	2.15	126.84	122.44
9	E	101[B]	6EJ	C23-N32-N31	2.13	120.83	119.77
9	E	101[A]	6EJ	C4-C5-C6	2.11	126.76	122.44
9	E	101[A]	6EJ	C23-N32-N31	2.07	120.80	119.77
9	E	101[B]	6EJ	C12-C14-N15	2.04	116.23	113.30

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	502	GOL	O1-C1-C2-C3
7	C	503[A]	GOL	O1-C1-C2-C3
7	C	503[B]	GOL	O1-C1-C2-C3
7	C	504	GOL	O1-C1-C2-C3
9	E	101[B]	6EJ	C17-C18-N21-C22
9	E	101[B]	6EJ	C12-C14-N15-C16
7	C	504	GOL	O1-C1-C2-O2
7	C	505	GOL	O1-C1-C2-O2
7	A	501	GOL	O1-C1-C2-C3
7	A	501	GOL	C1-C2-C3-O3
7	C	502	GOL	O1-C1-C2-C3
7	C	503[A]	GOL	C1-C2-C3-O3
7	C	505	GOL	O1-C1-C2-C3
7	A	501	GOL	O2-C2-C3-O3
7	C	503[A]	GOL	O1-C1-C2-O2
7	C	503[A]	GOL	O2-C2-C3-O3
7	C	503[B]	GOL	O1-C1-C2-O2
7	A	502	GOL	O1-C1-C2-O2
7	A	505	GOL	O2-C2-C3-O3
7	C	502	GOL	O1-C1-C2-O2
7	A	505	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	E	101[A]	6EJ	N21-C22-C23-N32
9	E	101[B]	6EJ	C19-C18-N21-C22
9	E	101[B]	6EJ	N21-C22-C23-C24
9	E	101[B]	6EJ	N21-C22-C23-N32
9	E	101[A]	6EJ	N21-C22-C23-C24
7	A	505	GOL	O1-C1-C2-C3
7	A	505	GOL	C1-C2-C3-O3
7	C	505	GOL	C1-C2-C3-O3

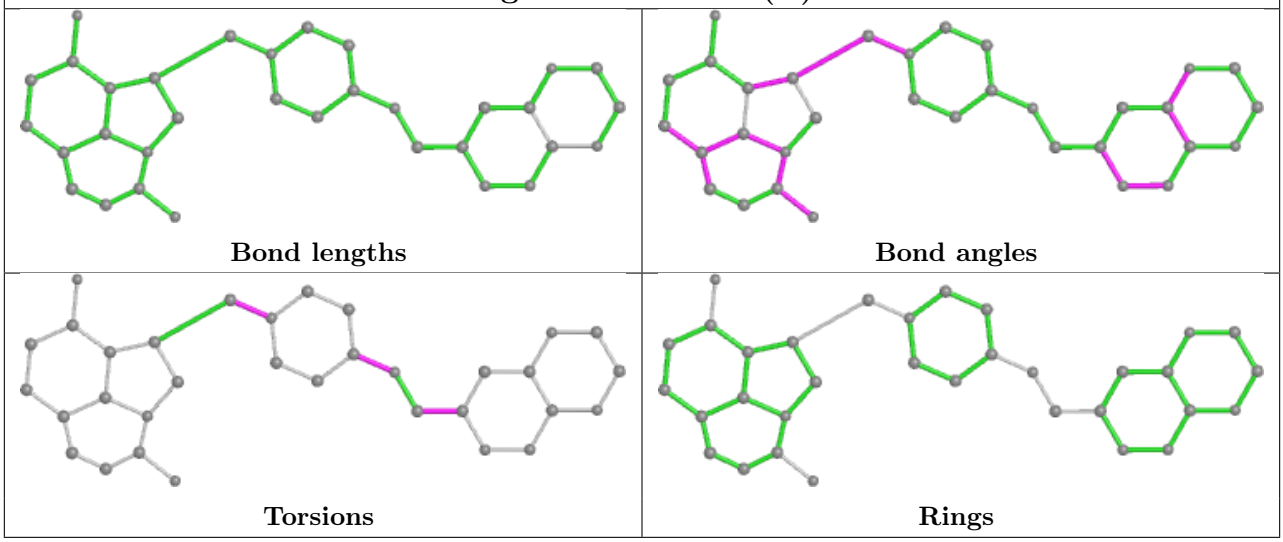
There are no ring outliers.

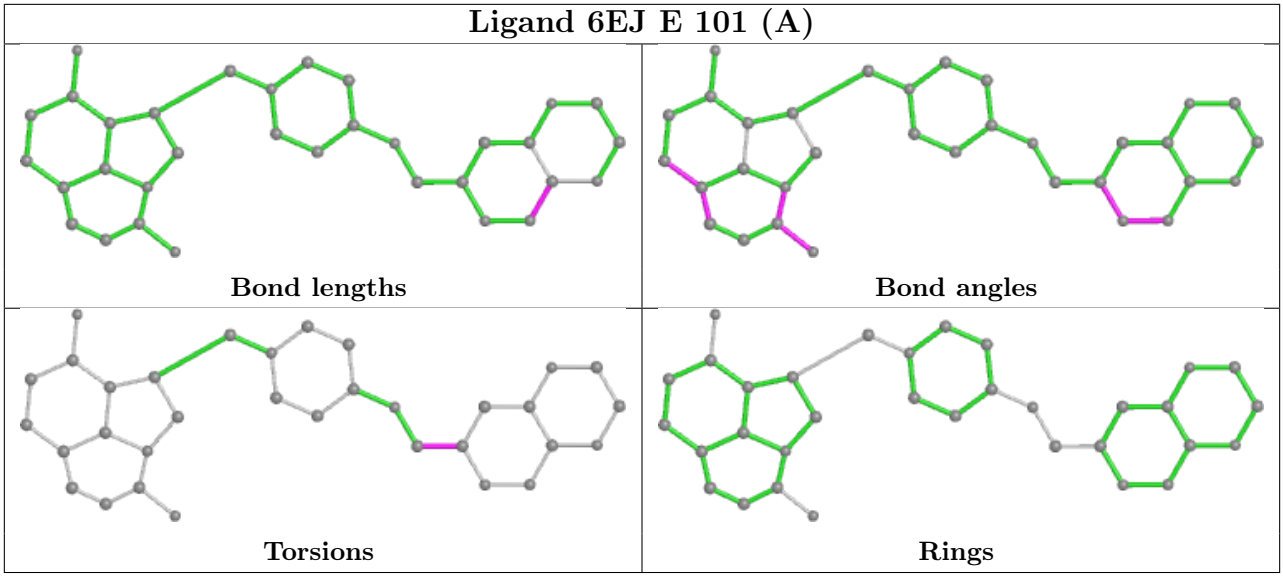
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	503[A]	GOL	1	0
9	E	101[A]	6EJ	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 6EJ E 101 (B)





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	192/202 (95%)	0.24	12 (6%)	20	22	25, 38, 59, 96	0
1	D	189/202 (93%)	0.45	13 (6%)	16	18	28, 43, 66, 82	0
2	A	483/490 (98%)	-0.16	9 (1%)	66	68	22, 32, 50, 78	0
2	C	481/490 (98%)	-0.23	4 (0%)	86	87	22, 31, 46, 71	0
3	E	20/20 (100%)	-0.34	0	100	100	22, 29, 47, 48	1 (5%)
4	F	8/8 (100%)	-0.36	0	100	100	25, 30, 42, 45	0
5	G	12/12 (100%)	-0.39	0	100	100	23, 34, 40, 45	1 (8%)
All	All	1385/1424 (97%)	-0.05	38 (2%)	54	56	22, 34, 55, 96	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	640	ALA	10.0
1	D	581[A]	LYS	6.5
1	B	416	GLY	5.6
1	B	639[A]	TYR	5.0
1	D	638	VAL	5.0
1	B	415	PRO	4.9
1	D	491	GLY	4.7
1	D	544	THR	4.7
2	C	490	LEU	3.9
1	B	638[A]	VAL	3.8
1	B	544	THR	3.8
1	D	424	LYS	3.7
1	B	491	GLY	3.6
1	B	612	ILE	3.6
1	D	612	ILE	3.5
2	A	9	ILE	3.5
1	B	545	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	469	LEU	3.1
1	D	470[A]	ASP	3.1
2	C	436	LEU	2.8
1	D	468[A]	ARG	2.8
1	B	427[A]	GLU	2.8
2	A	436	LEU	2.6
1	D	427[A]	GLU	2.5
2	A	402[A]	ASP	2.5
2	A	490	LEU	2.4
2	C	284	LYS	2.4
1	D	600	HIS	2.4
2	C	10	ASN	2.3
1	B	600	HIS	2.3
1	D	639	TYR	2.2
1	B	599[A]	GLU	2.1
1	D	621	LEU	2.1
2	A	439	ASP	2.1
2	A	300	THR	2.1
2	A	195	VAL	2.1
2	A	284	LYS	2.0
2	A	306	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	A	505	6/6	0.84	0.35	61,67,74,74	0
7	GOL	C	504	6/6	0.84	0.22	46,56,58,65	0

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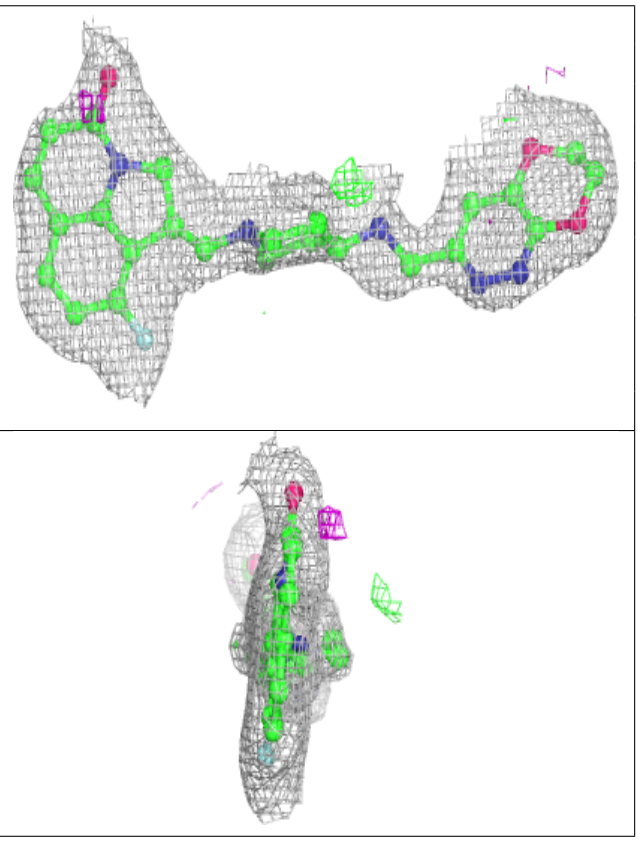
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	C	505	6/6	0.87	0.11	40,53,57,59	0
7	GOL	A	501	6/6	0.90	0.12	51,54,58,59	0
7	GOL	A	503	6/6	0.91	0.13	53,59,59,62	0
7	GOL	A	506	6/6	0.91	0.13	46,62,67,70	0
7	GOL	A	504	6/6	0.92	0.15	48,51,52,54	0
7	GOL	C	503[A]	6/6	0.93	0.14	40,44,47,49	6
7	GOL	C	503[B]	6/6	0.93	0.14	40,41,42,43	6
7	GOL	A	502	6/6	0.94	0.12	30,44,45,47	0
7	GOL	C	502	6/6	0.95	0.10	27,42,48,48	0
9	6EJ	E	101[A]	33/33	0.96	0.14	32,35,45,45	33
9	6EJ	E	101[B]	33/33	0.96	0.14	29,31,34,35	33
6	MN	D	1001[B]	1/1	0.98	0.08	26,26,26,26	1
6	MN	C	501	1/1	0.98	0.14	75,75,75,75	0
6	MN	D	1001[A]	1/1	0.98	0.08	32,32,32,32	1
8	CL	A	507	1/1	0.99	0.12	39,39,39,39	0
6	MN	B	701[A]	1/1	0.99	0.06	24,24,24,24	1
6	MN	B	701[B]	1/1	0.99	0.06	33,33,33,33	1

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.

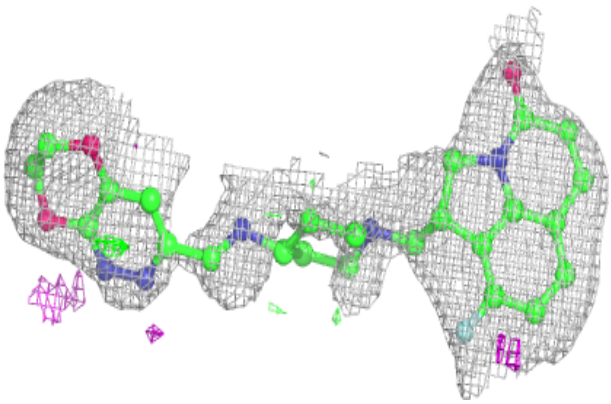
Electron density around 6EJ E 101 (A):

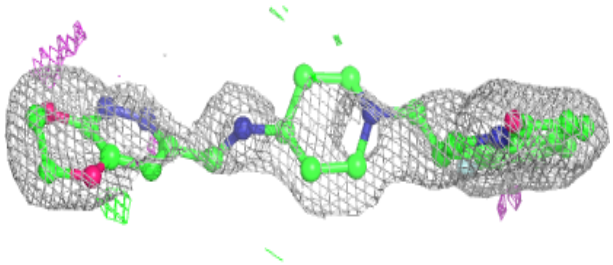
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

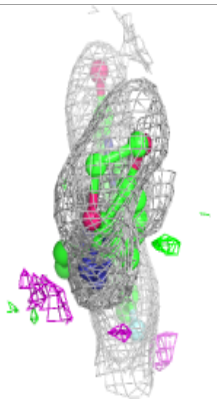


Electron density around 6EJ E 101 (B):

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







6.5 Other polymers (i)

There are no such residues in this entry.