wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2024 – 06:18 PM EST

PDB ID	:	4K4G
Title	:	Ternary crystal structures of human DNA POLYMERASE LAMBDA IN COMPLEX WITH DNA AND L-DCTP.
Authors	:	Vyas, R.; Suo, Z.
Deposited on	:	2013-04-12
Resolution	:	2.15 Å(reported)

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

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

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

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

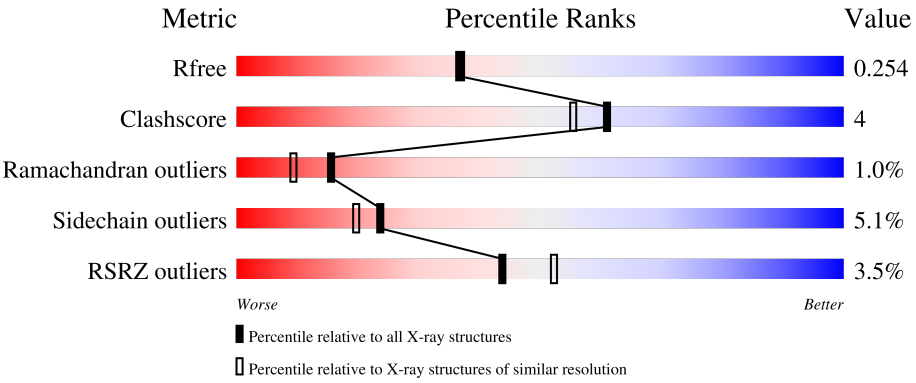
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	A	340	2% 81% 12% • 5%
1	E	340	4% 78% 15% • 5%
1	I	340	5% 86% 9% • •
1	M	340	3% 81% 13% • • •
2	B	11	64% 36%

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Mol	Chain	Length	Quality of chain
2	F	11	45% 55%
2	J	11	100%
2	N	11	73% 27%
3	C	6	100%
3	G	6	83% 17%
3	K	6	100%
3	O	6	100%
4	D	4	25% 75%
4	H	4	75% 25%
4	L	4	75% 25%
4	P	4	75% 25%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12538 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 polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2548	1603	466	468	11			
1	E	323	Total	C	N	O	S	0	0	0
			2541	1600	466	463	12			
1	I	327	Total	C	N	O	S	0	0	0
			2580	1621	474	473	12			
1	M	328	Total	C	N	O	S	0	0	0
			2584	1624	474	474	12			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	MET	-	expression tag	UNP Q9UGP5
A	576	LEU	-	expression tag	UNP Q9UGP5
A	577	GLU	-	expression tag	UNP Q9UGP5
A	578	HIS	-	expression tag	UNP Q9UGP5
A	579	HIS	-	expression tag	UNP Q9UGP5
A	580	HIS	-	expression tag	UNP Q9UGP5
A	581	HIS	-	expression tag	UNP Q9UGP5
A	582	HIS	-	expression tag	UNP Q9UGP5
A	583	HIS	-	expression tag	UNP Q9UGP5
E	244	MET	-	expression tag	UNP Q9UGP5
E	576	LEU	-	expression tag	UNP Q9UGP5
E	577	GLU	-	expression tag	UNP Q9UGP5
E	578	HIS	-	expression tag	UNP Q9UGP5
E	579	HIS	-	expression tag	UNP Q9UGP5
E	580	HIS	-	expression tag	UNP Q9UGP5
E	581	HIS	-	expression tag	UNP Q9UGP5
E	582	HIS	-	expression tag	UNP Q9UGP5
E	583	HIS	-	expression tag	UNP Q9UGP5
I	244	MET	-	expression tag	UNP Q9UGP5
I	576	LEU	-	expression tag	UNP Q9UGP5
I	577	GLU	-	expression tag	UNP Q9UGP5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	578	HIS	-	expression tag	UNP Q9UGP5
I	579	HIS	-	expression tag	UNP Q9UGP5
I	580	HIS	-	expression tag	UNP Q9UGP5
I	581	HIS	-	expression tag	UNP Q9UGP5
I	582	HIS	-	expression tag	UNP Q9UGP5
I	583	HIS	-	expression tag	UNP Q9UGP5
M	244	MET	-	expression tag	UNP Q9UGP5
M	576	LEU	-	expression tag	UNP Q9UGP5
M	577	GLU	-	expression tag	UNP Q9UGP5
M	578	HIS	-	expression tag	UNP Q9UGP5
M	579	HIS	-	expression tag	UNP Q9UGP5
M	580	HIS	-	expression tag	UNP Q9UGP5
M	581	HIS	-	expression tag	UNP Q9UGP5
M	582	HIS	-	expression tag	UNP Q9UGP5
M	583	HIS	-	expression tag	UNP Q9UGP5

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*GP*CP*GP*GP*TP*AP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			
2	F	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			
2	J	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			
2	N	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			

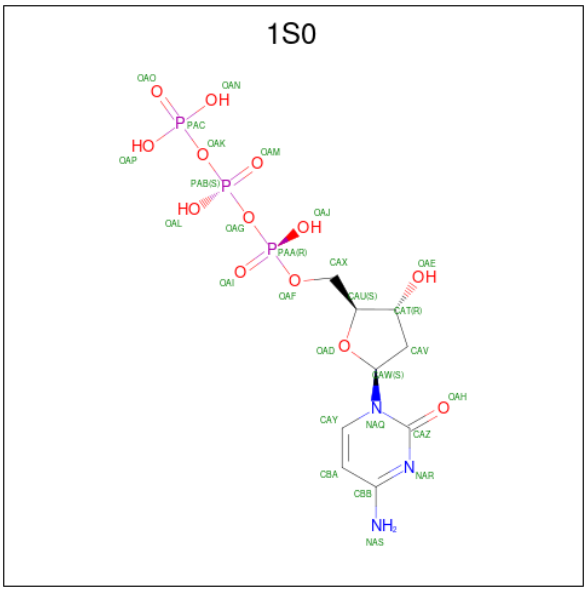
- Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*GP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			
3	G	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			
3	K	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			
3	O	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
4	H	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
4	L	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
4	P	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

- Molecule 5 is 4-amino-1-{2-deoxy-5-O-[(R)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-L-erythro-pentofuranosyl}pyrimidin-2(1H)-one (three-letter code: 1S0) (formula: $C_9H_{16}N_3O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
5	E	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
5	I	1	Total	C	N	O	P	0	0
			28	9	3	13	3		
5	M	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	Ca	0	0
			5	5		

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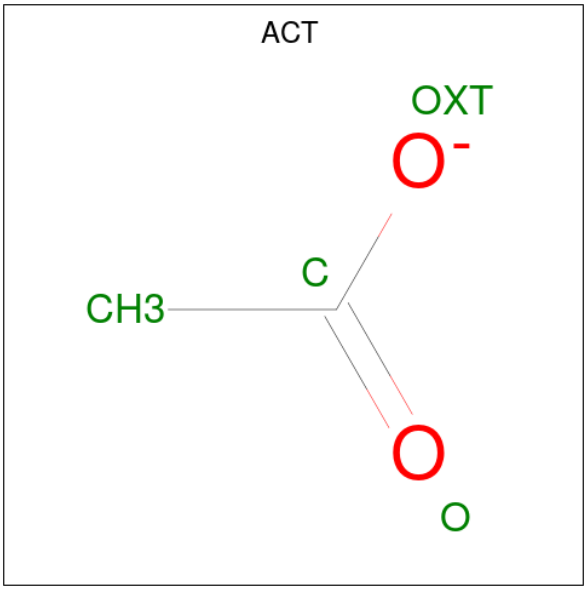
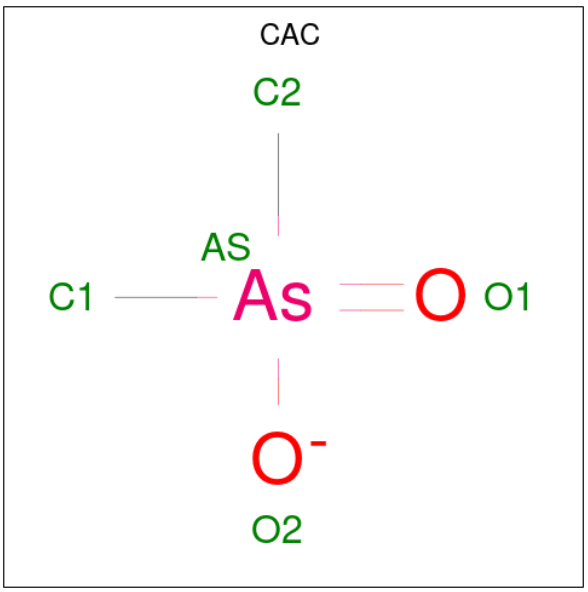
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0
6	E	5	Total Ca 5 5	0	0
6	F	1	Total Ca 1 1	0	0
6	I	3	Total Ca 3 3	0	0
6	J	2	Total Ca 2 2	0	0
6	L	1	Total Ca 1 1	0	0
6	M	4	Total Ca 4 4	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	I	1	Total C O 4 2 2	0	0
7	M	1	Total C O 4 2 2	0	0

- Molecule 8 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total As C O 5 1 2 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	112	Total O 112 112	0	0
9	B	21	Total O 21 21	0	0
9	C	11	Total O 11 11	0	0
9	E	64	Total O 64 64	0	0
9	F	7	Total O 7 7	0	0
9	G	4	Total O 4 4	0	0
9	H	1	Total O 1 1	0	0
9	I	66	Total O 66 66	0	0
9	J	5	Total O 5 5	0	0
9	K	14	Total O 14 14	0	0

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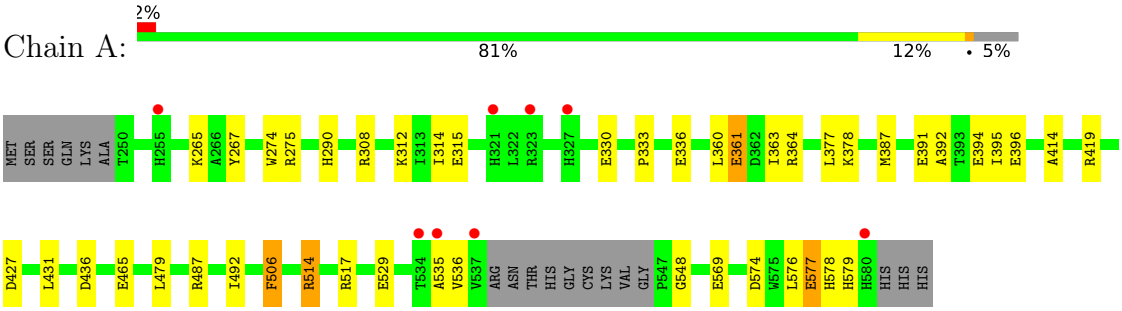
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total O 1 1	0	0
9	M	105	Total O 105 105	0	0
9	N	7	Total O 7 7	0	0
9	O	2	Total O 2 2	0	0
9	P	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

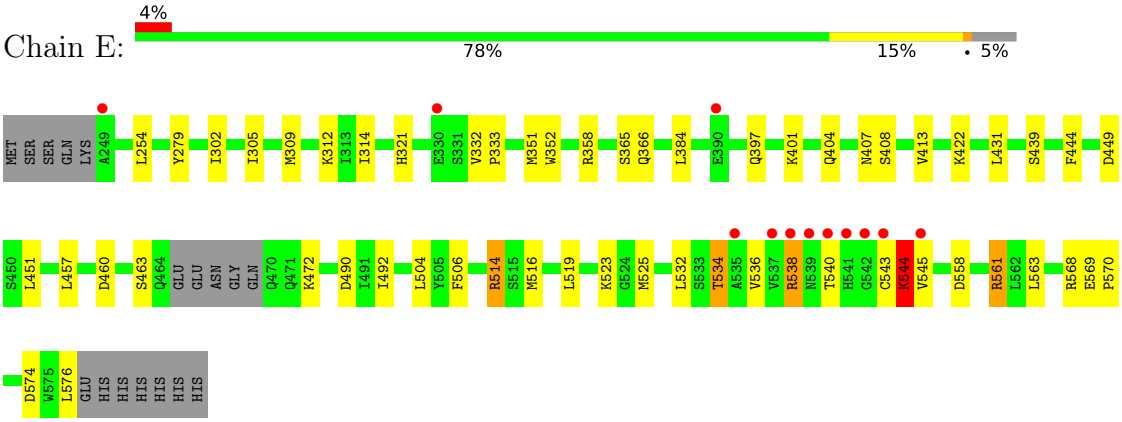
• Molecule 1: DNA polymerase lambda

Chain A:



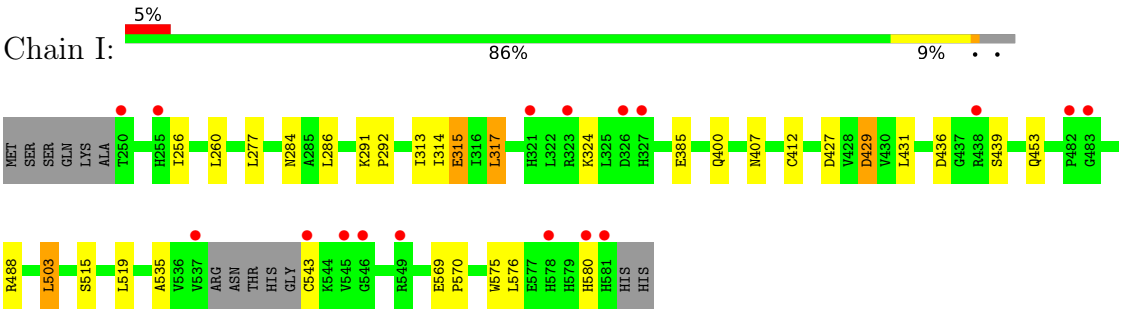
• Molecule 1: DNA polymerase lambda

Chain E:



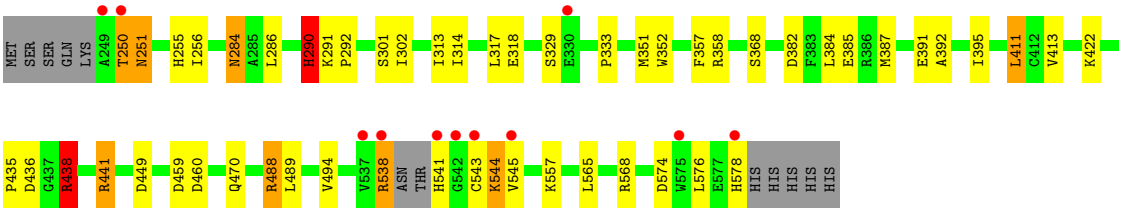
• Molecule 1: DNA polymerase lambda

Chain I:



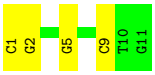
• Molecule 1: DNA polymerase lambda

Chain M:



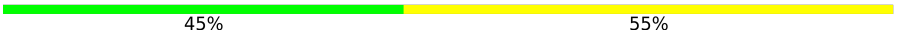
• Molecule 2: DNA (5’-D(*CP*GP*GP*CP*GP*GP*TP*AP*CP*TP*G)-3’)

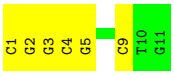
Chain B:



• Molecule 2: DNA (5’-D(*CP*GP*GP*CP*GP*GP*TP*AP*CP*TP*G)-3’)

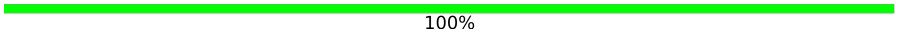
Chain F:





• Molecule 2: DNA (5’-D(*CP*GP*GP*CP*GP*GP*TP*AP*CP*TP*G)-3’)

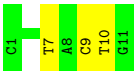
Chain J:



There are no outlier residues recorded for this chain.

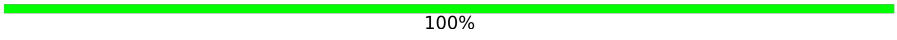
• Molecule 2: DNA (5’-D(*CP*GP*GP*CP*GP*GP*TP*AP*CP*TP*G)-3’)

Chain N:



• Molecule 3: DNA (5’-D(*CP*AP*GP*TP*AP*C)-3’)

Chain C:



There are no outlier residues recorded for this chain.

• Molecule 3: DNA (5’-D(*CP*AP*GP*TP*AP*C)-3’)

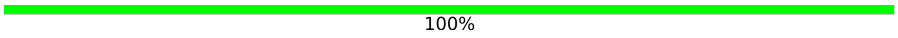
Chain G:

• Molecule 3: DNA (5’-D(*CP*AP*GP*TP*AP*C)-3’)

Chain K: 

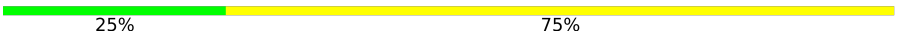
There are no outlier residues recorded for this chain.

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

Chain O: 

There are no outlier residues recorded for this chain.

• Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain D: 

• Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain H: 

• Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain L: 

• Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain P: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	194.57Å 97.81Å 105.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.60 – 2.15 36.60 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.1 (36.60-2.15) 98.1 (36.60-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.200 , 0.250 0.206 , 0.254	Depositor DCC
R_{free} test set	5379 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12538	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1S0, CAC, CA, ACT

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	A	0.90	1/2602 (0.0%)	0.95	8/3511 (0.2%)
1	E	0.77	0/2593	0.89	4/3499 (0.1%)
1	I	0.78	1/2635 (0.0%)	0.84	4/3555 (0.1%)
1	M	0.86	0/2637	1.03	7/3557 (0.2%)
2	B	0.71	0/252	0.91	0/388
2	F	0.52	0/252	1.00	1/388 (0.3%)
2	J	0.68	0/252	1.02	0/388
2	N	0.76	0/252	0.90	0/388
3	C	0.77	0/133	0.84	0/203
3	G	0.69	0/133	1.04	2/203 (1.0%)
3	K	0.71	0/133	1.00	0/203
3	O	0.71	0/133	0.91	0/203
4	D	1.26	1/92 (1.1%)	1.04	1/138 (0.7%)
4	H	1.22	1/92 (1.1%)	0.80	0/138
4	L	1.11	1/92 (1.1%)	0.77	0/138
4	P	1.20	1/92 (1.1%)	0.96	1/138 (0.7%)
All	All	0.83	6/12375 (0.0%)	0.93	28/17038 (0.2%)

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	I	0	1
1	M	0	1
All	All	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	DG	OP3-P	-10.10	1.49	1.61
4	P	1	DG	OP3-P	-10.05	1.49	1.61
4	D	1	DG	OP3-P	-10.04	1.49	1.61
4	L	1	DG	OP3-P	-9.55	1.49	1.61
1	A	465	GLU	CD-OE2	6.78	1.33	1.25

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	488	ARG	NE-CZ-NH2	-15.05	112.77	120.30
1	M	488	ARG	NE-CZ-NH1	12.21	126.40	120.30
1	M	441	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	M	441	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	A	427	ASP	CB-CG-OD1	8.20	125.68	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	580	HIS	Peptide
1	M	290	HIS	Peptide

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	A	2548	0	2540	33	0
1	E	2541	0	2554	25	0
1	I	2580	0	2562	13	0
1	M	2584	0	2583	27	0
2	B	225	0	125	4	0
2	F	225	0	125	4	0
2	J	225	0	125	0	0
2	N	225	0	125	2	0
3	C	119	0	68	0	0
3	G	119	0	68	0	0
3	K	119	0	69	0	0
3	O	119	0	69	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	83	0	45	1	0
4	H	83	0	45	0	0
4	L	83	0	45	0	0
4	P	83	0	45	0	0
5	A	28	0	14	0	0
5	E	28	0	13	0	0
5	I	28	0	15	0	0
5	M	28	0	15	0	0
6	A	5	0	0	0	0
6	B	1	0	0	0	0
6	E	5	0	0	0	0
6	F	1	0	0	0	0
6	I	3	0	0	0	0
6	J	2	0	0	0	0
6	L	1	0	0	0	0
6	M	4	0	0	0	0
7	B	4	0	3	0	0
7	F	4	0	3	0	0
7	I	4	0	3	0	0
7	M	4	0	3	0	0
8	M	5	0	0	2	0
9	A	112	0	0	7	0
9	B	21	0	0	1	0
9	C	11	0	0	0	0
9	E	64	0	0	1	0
9	F	7	0	0	2	0
9	G	4	0	0	0	0
9	H	1	0	0	0	0
9	I	66	0	0	0	0
9	J	5	0	0	0	0
9	K	14	0	0	0	0
9	L	1	0	0	0	0
9	M	105	0	0	3	0
9	N	7	0	0	1	0
9	O	2	0	0	0	0
9	P	2	0	0	0	0
All	All	12538	0	11262	104	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 4.

The worst 5 of 104 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:543:CYS:HG	1:I:543:CYS:N	1.55	1.04
1:A:387:MET:HE1	1:A:395:ILE:HD12	1.61	0.83
2:B:9:DC:OP1	9:B:208:HOH:O	2.00	0.77
1:E:431:LEU:HD12	1:E:492:ILE:HG23	1.66	0.77
1:A:387:MET:CE	1:A:395:ILE:HD12	2.16	0.75

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	A	318/340 (94%)	307 (96%)	9 (3%)	2 (1%)	25 18
1	E	319/340 (94%)	303 (95%)	12 (4%)	4 (1%)	12 6
1	I	323/340 (95%)	313 (97%)	9 (3%)	1 (0%)	41 37
1	M	324/340 (95%)	304 (94%)	14 (4%)	6 (2%)	8 2
All	All	1284/1360 (94%)	1227 (96%)	44 (3%)	13 (1%)	15 9

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	HIS
1	M	251	ASN
1	I	535	ALA
1	M	301	SER
1	E	540	THR

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	A	272/287 (95%)	266 (98%)	6 (2%)	52 55
1	E	271/287 (94%)	252 (93%)	19 (7%)	15 10
1	I	274/287 (96%)	264 (96%)	10 (4%)	35 33
1	M	275/287 (96%)	254 (92%)	21 (8%)	13 8
All	All	1092/1148 (95%)	1036 (95%)	56 (5%)	24 20

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	317	LEU
1	M	578	HIS
1	M	250	THR
1	M	576	LEU
1	M	489	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	453	GLN
1	M	290	HIS
1	M	284	ASN
1	M	372	GLN
1	A	511	HIS

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 31 ligands modelled in this entry, 22 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	1S0	I	601	6	25,29,29	1.73	2 (8%)	37,45,45	1.53	4 (10%)
7	ACT	F	102	-	3,3,3	0.70	0	3,3,3	0.98	0
5	1S0	M	602	6	25,29,29	1.35	2 (8%)	37,45,45	1.81	7 (18%)
7	ACT	I	605	-	3,3,3	0.68	0	3,3,3	1.33	0
5	1S0	A	601	6	25,29,29	1.53	4 (16%)	37,45,45	1.29	4 (10%)
5	1S0	E	601	6	25,29,29	1.25	2 (8%)	37,45,45	1.55	5 (13%)
8	CAC	M	607	-	0,4,4	-	-	0,6,6	-	-
7	ACT	B	102	-	3,3,3	0.80	0	3,3,3	0.72	0
7	ACT	M	601	-	3,3,3	0.83	0	3,3,3	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1S0	A	601	6	-	3/22/34/34	0/2/2/2
5	1S0	M	602	6	-	1/22/34/34	0/2/2/2
5	1S0	I	601	6	-	1/22/34/34	0/2/2/2
5	1S0	E	601	6	-	4/22/34/34	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	601	1S0	OAH-CAZ	7.86	1.38	1.23
5	A	601	1S0	OAH-CAZ	5.46	1.33	1.23
5	M	602	1S0	OAH-CAZ	5.01	1.33	1.23
5	E	601	1S0	OAH-CAZ	4.36	1.31	1.23
5	M	602	1S0	CAY-CBA	2.74	1.41	1.35

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	602	1S0	OAH-CAZ-NAR	-5.45	113.46	122.33
5	I	601	1S0	OAH-CAZ-NAR	-5.31	113.69	122.33
5	M	602	1S0	OAD-CAW-NAQ	4.63	116.14	107.86
5	E	601	1S0	OAH-CAZ-NAR	-4.52	114.98	122.33
5	A	601	1S0	OAH-CAZ-NAR	-4.42	115.15	122.33

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	1S0	PAB-OAK-PAC-OAP
5	E	601	1S0	PAB-OAK-PAC-OAP
5	I	601	1S0	PAB-OAG-PAA-OAF
5	M	602	1S0	PAB-OAG-PAA-OAF
5	E	601	1S0	PAA-OAG-PAB-OAM

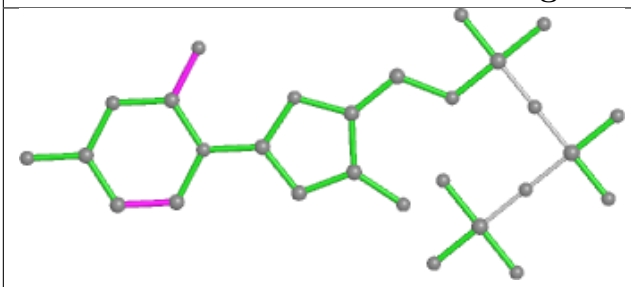
There are no ring outliers.

1 monomer is involved in 2 short contacts:

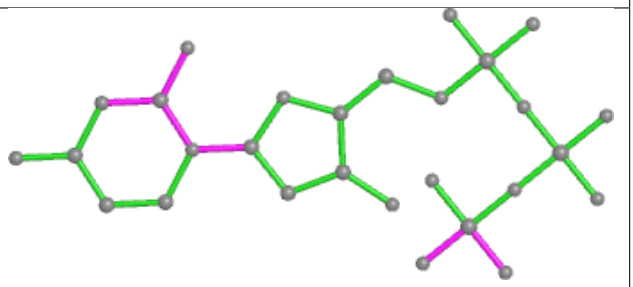
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	607	CAC	2	0

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 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.

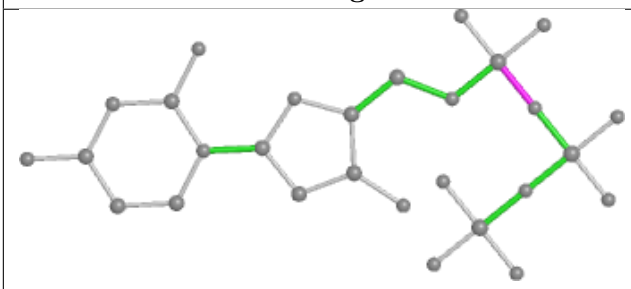
Ligand 1S0 I 601



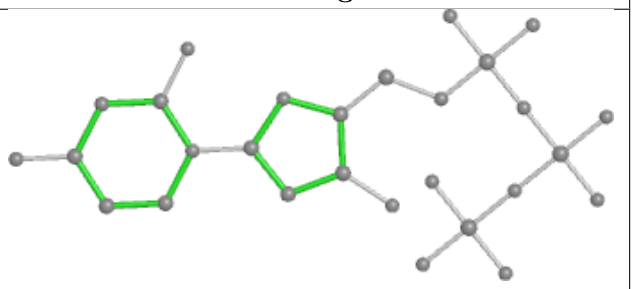
Bond lengths



Bond angles

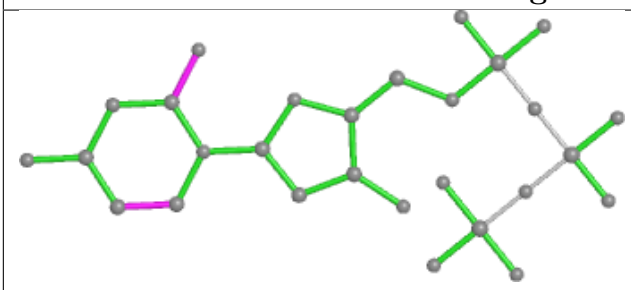


Torsions

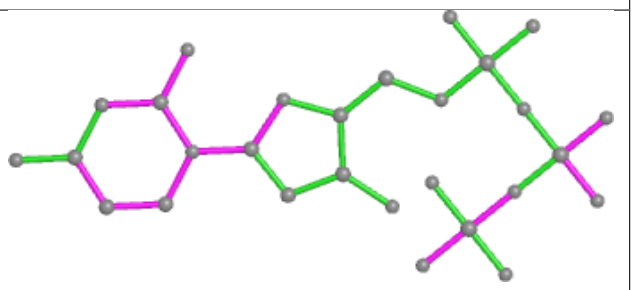


Rings

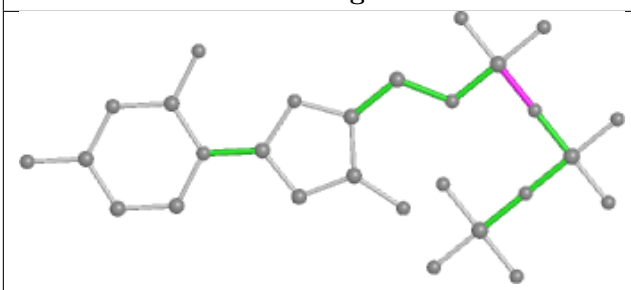
Ligand 1S0 M 602



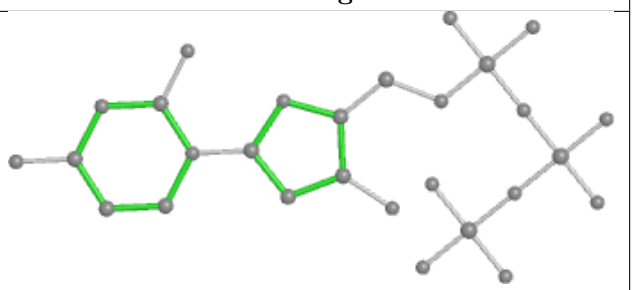
Bond lengths



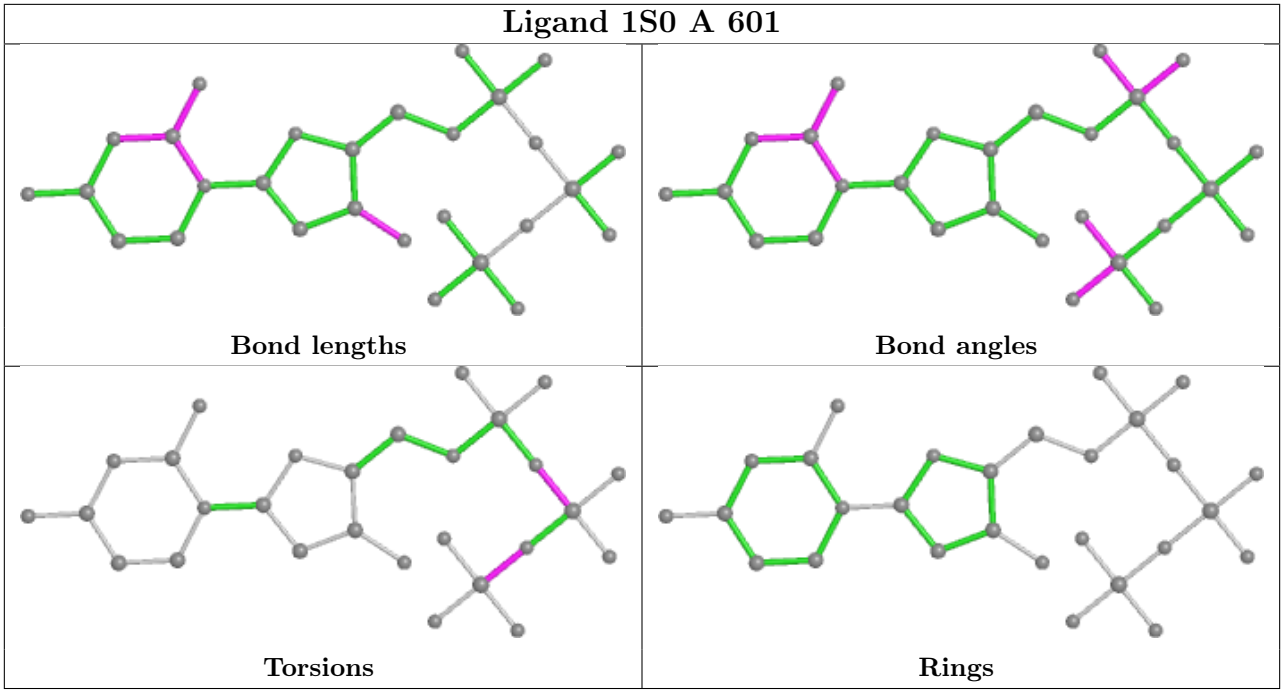
Bond angles

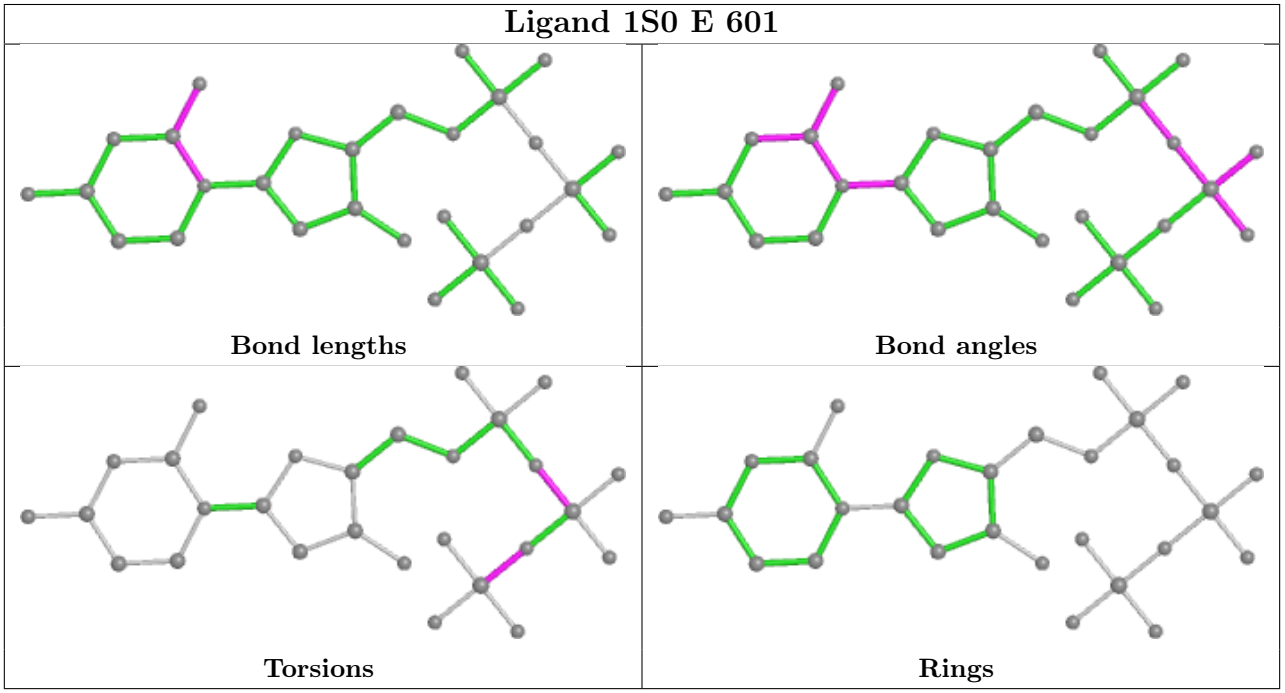


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	322/340 (94%)	-0.04	8 (2%) 57 65	17, 34, 60, 112	0
1	E	323/340 (95%)	0.00	12 (3%) 41 49	20, 40, 70, 118	0
1	I	327/340 (96%)	0.10	17 (5%) 27 35	22, 42, 70, 104	0
1	M	328/340 (96%)	0.13	11 (3%) 45 53	17, 38, 60, 104	0
2	B	11/11 (100%)	-0.21	0 100 100	21, 26, 44, 44	0
2	F	11/11 (100%)	-0.29	0 100 100	38, 43, 54, 62	0
2	J	11/11 (100%)	-0.44	0 100 100	36, 40, 43, 50	0
2	N	11/11 (100%)	-0.38	0 100 100	24, 32, 42, 50	0
3	C	6/6 (100%)	-0.23	0 100 100	19, 23, 38, 43	0
3	G	6/6 (100%)	-0.03	0 100 100	32, 35, 62, 73	0
3	K	6/6 (100%)	-0.27	0 100 100	25, 29, 55, 57	0
3	O	6/6 (100%)	-0.35	0 100 100	28, 32, 52, 59	0
4	D	4/4 (100%)	-0.58	0 100 100	33, 35, 38, 39	0
4	H	4/4 (100%)	-0.63	0 100 100	32, 34, 38, 44	0
4	L	4/4 (100%)	-0.43	0 100 100	44, 46, 51, 51	0
4	P	4/4 (100%)	-0.50	0 100 100	34, 38, 45, 47	0
All	All	1384/1444 (95%)	0.03	48 (3%) 44 52	17, 38, 67, 118	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	540	THR	8.5
1	M	249	ALA	7.8
1	E	541	HIS	6.9
1	A	580	HIS	6.1
1	I	543	CYS	5.9

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	J	102	1/1	0.48	0.15	81,81,81,81	0
6	CA	E	604	1/1	0.54	0.34	78,78,78,78	0
6	CA	E	605	1/1	0.72	0.11	56,56,56,56	0
6	CA	I	602	1/1	0.73	0.14	69,69,69,69	0
6	CA	M	604	1/1	0.73	0.13	72,72,72,72	0
6	CA	I	603	1/1	0.75	0.13	77,77,77,77	0
6	CA	M	606	1/1	0.82	0.18	72,72,72,72	0
6	CA	M	603	1/1	0.83	0.06	67,67,67,67	0
7	ACT	I	605	4/4	0.85	0.26	46,53,55,55	0
6	CA	J	101	1/1	0.86	0.12	67,67,67,67	0
6	CA	A	605	1/1	0.86	0.15	57,57,57,57	0
5	1S0	I	601	28/28	0.88	0.18	51,76,84,84	0
8	CAC	M	607	5/5	0.89	0.16	96,106,107,123	0
7	ACT	B	102	4/4	0.90	0.14	60,62,63,71	0
7	ACT	M	601	4/4	0.92	0.22	54,58,61,64	0
5	1S0	M	602	28/28	0.93	0.12	31,47,58,61	0
6	CA	F	101	1/1	0.93	0.05	56,56,56,56	0
7	ACT	F	102	4/4	0.93	0.20	45,51,53,57	0
6	CA	M	605	1/1	0.94	0.13	40,40,40,40	0
6	CA	B	101	1/1	0.95	0.07	59,59,59,59	0
6	CA	L	101	1/1	0.97	0.10	78,78,78,78	0
5	1S0	E	601	28/28	0.97	0.11	23,30,39,43	0
6	CA	A	604	1/1	0.97	0.17	34,34,34,34	0
6	CA	E	606	1/1	0.97	0.19	41,41,41,41	0
6	CA	E	603	1/1	0.97	0.05	37,37,37,37	0
6	CA	E	602	1/1	0.98	0.07	34,34,34,34	0
6	CA	A	603	1/1	0.98	0.09	20,20,20,20	0

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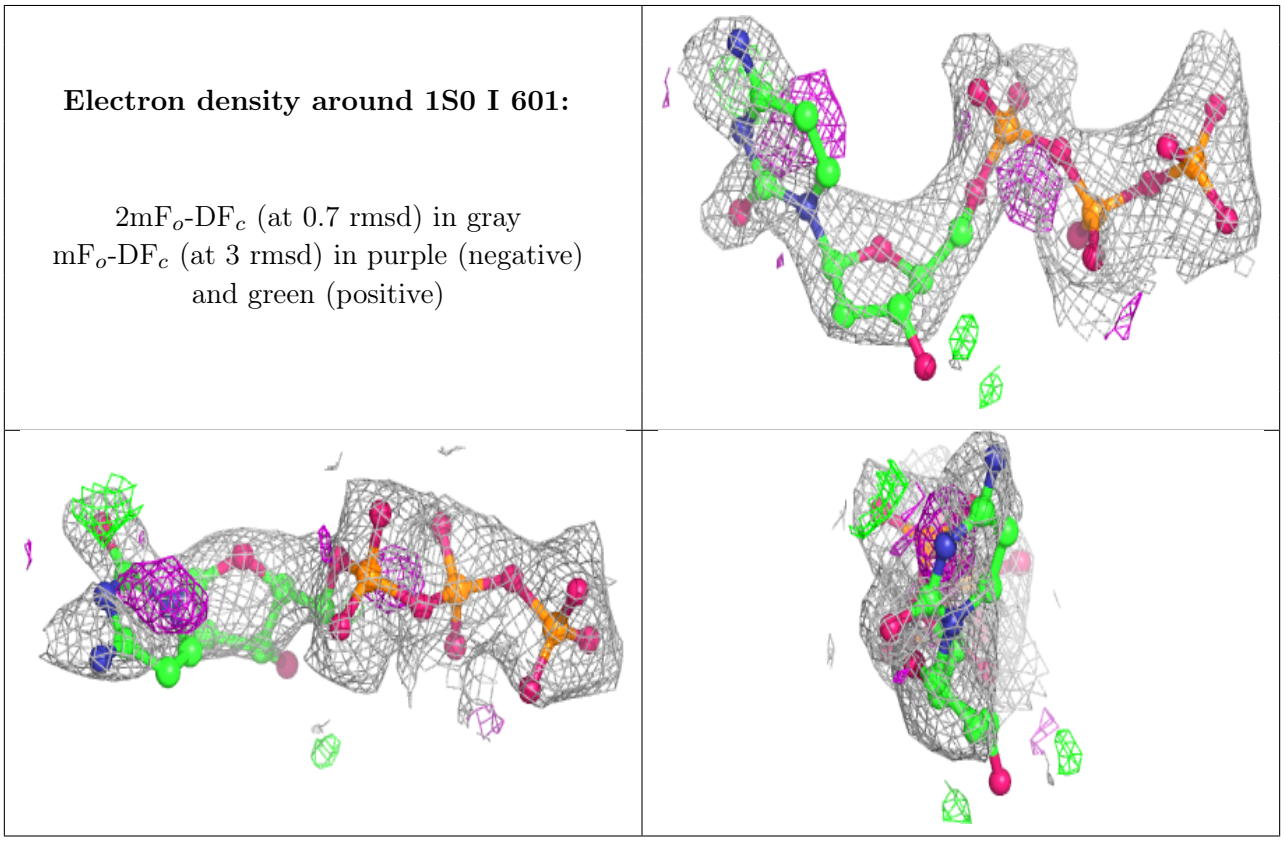
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	I	604	1/1	0.98	0.09	20,20,20,20	1
5	1S0	A	601	28/28	0.99	0.13	14,18,21,23	0
6	CA	A	606	1/1	0.99	0.05	42,42,42,42	0
6	CA	A	602	1/1	0.99	0.10	20,20,20,20	0

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.

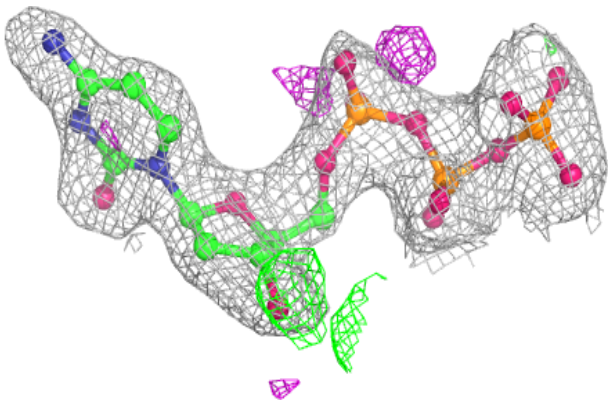
Electron density around 1S0 I 601:

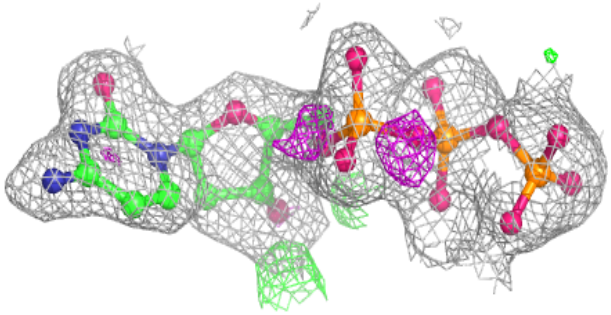
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

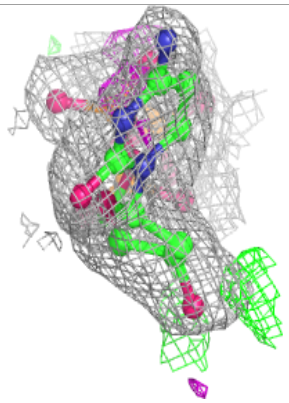


Electron density around 1S0 M 602:

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

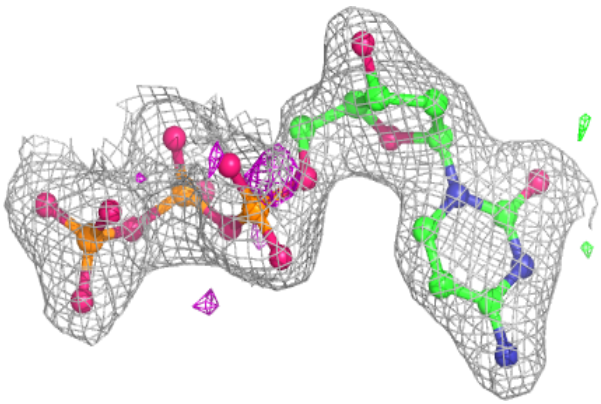


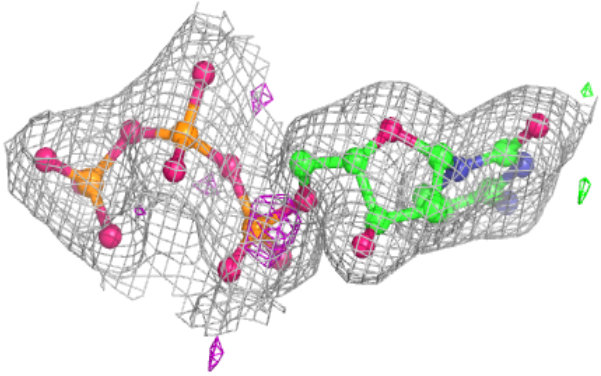


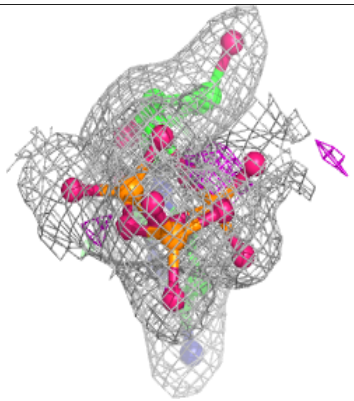


Electron density around 1S0 E 601:

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

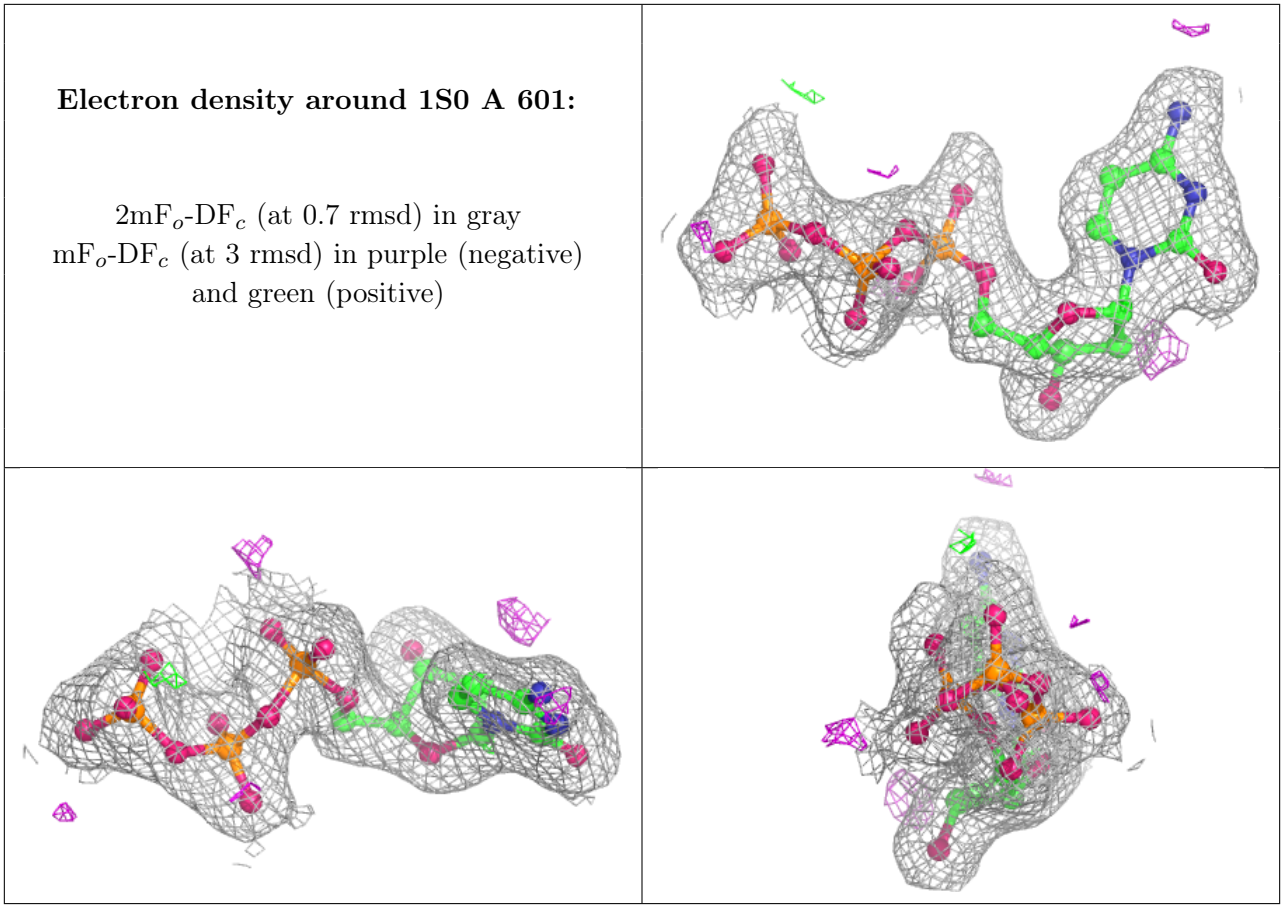






Electron density around 1S0 A 601:

$2mF_o$-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

There are no such residues in this entry.