



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:45 pm BST

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 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

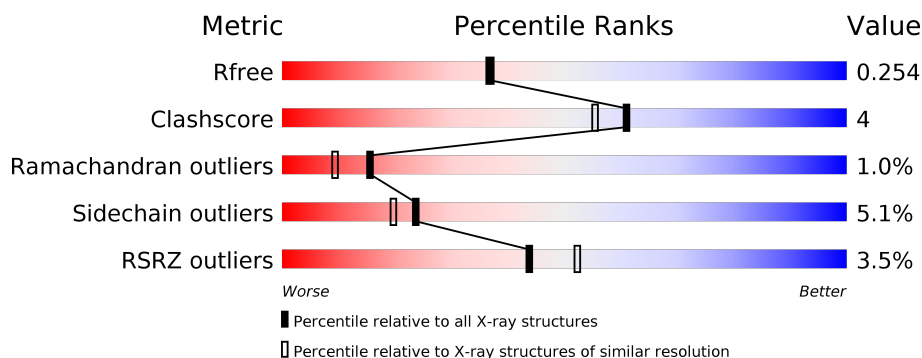
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 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	A	340	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>5%</div> </div> </div>
1	E	340	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>5%</div> </div> </div>
1	I	340	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>•</div> </div> </div>
1	M	340	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• • •</div> </div> </div>
2	B	11	<div> <div></div> <div> <div>64%</div> <div>36%</div> </div> </div>
2	F	11	<div> <div></div> <div> <div>45%</div> <div>55%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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

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			

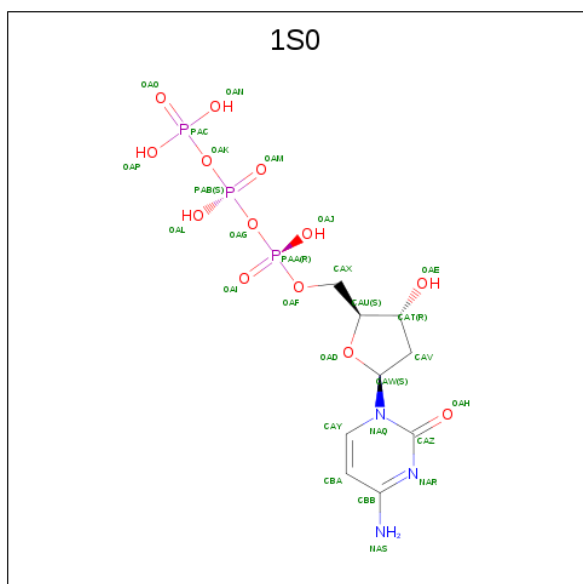
- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*AP\*GP\*TP\*AP\*C)-3').

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 83	C 38	N 16	O 25	P 4	0	0	0
4	H	4	Total 83	C 38	N 16	O 25	P 4	0	0	0
4	L	4	Total 83	C 38	N 16	O 25	P 4	0	0	0
4	P	4	Total 83	C 38	N 16	O 25	P 4	0	0	0

- 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:  $\text{C}_9\text{H}_{16}\text{N}_3\text{O}_{13}\text{P}_3$ ).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	2	Total Ca 2 2	0	0

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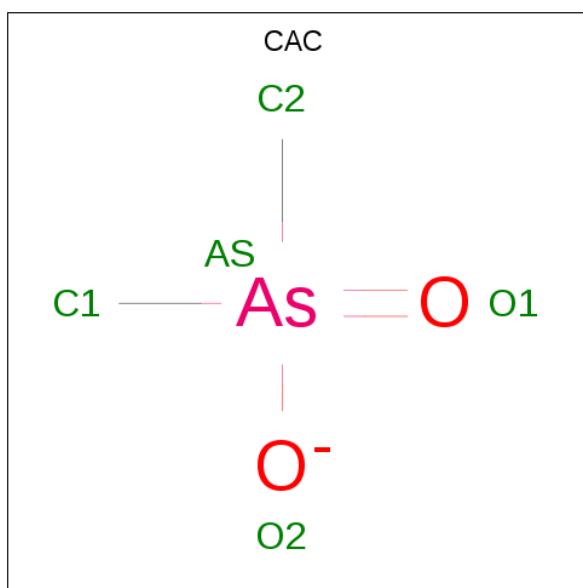
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	5	Total 5	Ca 5	0	0
6	B	1	Total 1	Ca 1	0	0
6	I	3	Total 3	Ca 3	0	0
6	A	5	Total 5	Ca 5	0	0
6	L	1	Total 1	Ca 1	0	0
6	F	1	Total 1	Ca 1	0	0
6	M	4	Total 4	Ca 4	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0
7	I	1	Total 4	C 2	O 2	0	0
7	M	1	Total 4	C 2	O 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	0	0
			5	1	2	2		

- Molecule 9 is water.

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

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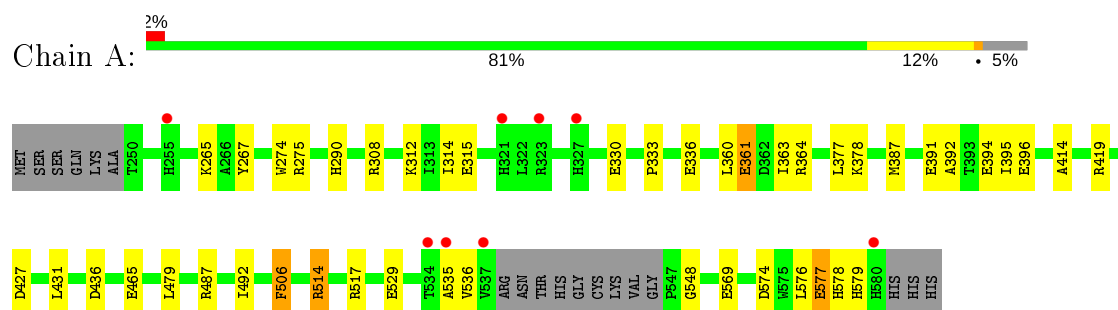
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	1	Total 1	O 1	0	0
9	M	105	Total 105	O 105	0	0
9	N	7	Total 7	O 7	0	0
9	O	2	Total 2	O 2	0	0
9	P	2	Total 2	O 2	0	0

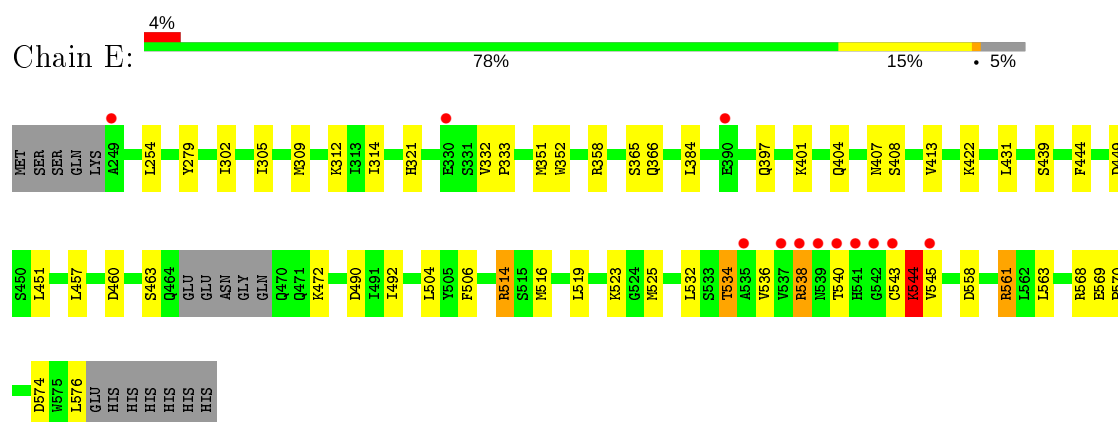
### 3 Residue-property plots [i](#)

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.

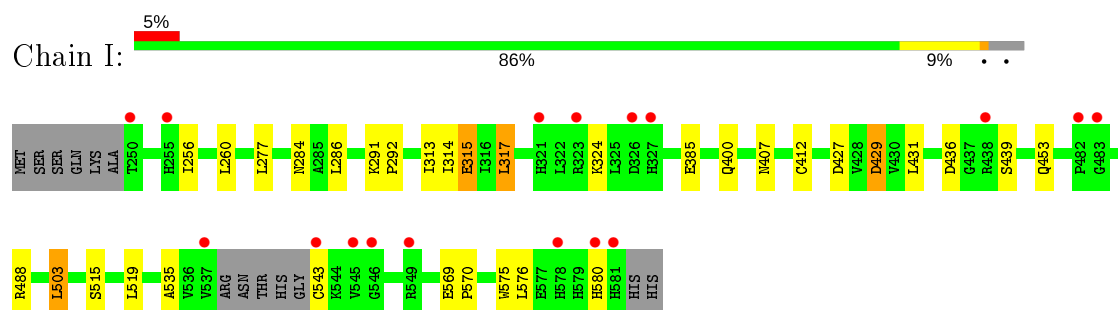
- Molecule 1: DNA polymerase lambda



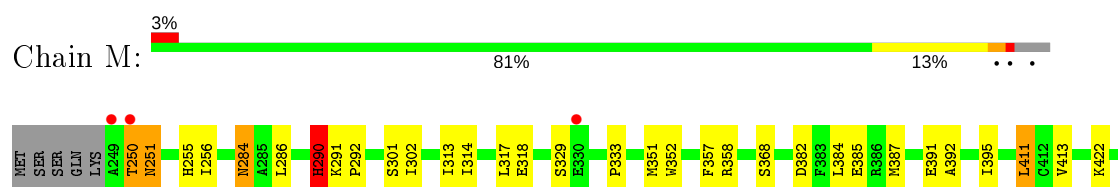
- Molecule 1: DNA polymerase lambda



- Molecule 1: DNA polymerase lambda



- Molecule 1: DNA polymerase lambda



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



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

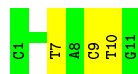


- Molecule 2: DNA (5'-D(\*CP\*GP\*GP\*CP\*GP\*GP\*TP\*AP\*CP\*TP\*G)-3')



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')

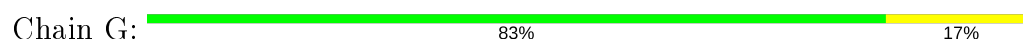


- Molecule 3: DNA (5'-D(\*CP\*AP\*GP\*TP\*AP\*C)-3')



There are no outlier residues recorded for this chain.

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



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

Chain K:  100%

There are no outlier residues recorded for this chain.

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

Chain O:  100%

There are no outlier residues recorded for this chain.

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

Chain D:  25% 75%



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

Chain H:  75% 25%



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

Chain L:  75% 25%



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

Chain P:  75% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

All (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
1	I	429	ASP	CB-CG	5.61	1.63	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	517	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	I	429	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	419	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	436	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	I	488	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	M	438	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	I	427	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	517	ARG	NE-CZ-NH2	-6.07	117.26	120.30
4	D	1	DG	O5'-P-OP1	-5.90	100.39	105.70
1	E	358	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	436	ASP	CB-CG-OD1	5.80	123.52	118.30
2	F	4	DC	C1'-O4'-C4'	-5.52	104.58	110.10
1	E	490	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	561	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	487	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	E	460	ASP	CB-CG-OD1	5.35	123.12	118.30
1	M	459	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	I	488	ARG	NE-CZ-NH1	5.13	122.86	120.30
3	G	1	DC	C5'-C4'-O4'	5.08	118.96	109.30
4	P	1	DG	O5'-P-OP1	-5.08	101.13	105.70
1	M	460	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	514	ARG	NE-CZ-NH2	-5.03	117.79	120.30
3	G	1	DC	C5'-C4'-C3'	5.02	123.14	114.10

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

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:N:7:DT:OP2	9:N:205:HOH:O	2.05	0.74
1:A:535:ALA:HB3	1:A:548:GLY:HA2	1.67	0.74
1:A:396:GLU:HG3	1:A:414:ALA:HB2	1.70	0.74
2:F:3:DG:N3	9:F:202:HOH:O	2.24	0.70
1:M:387:MET:HE1	1:M:395:ILE:HD12	1.73	0.69
1:E:543:CYS:SG	1:I:543:CYS:N	2.65	0.69
1:A:579:HIS:HB3	9:A:730:HOH:O	1.92	0.67
1:M:333:PRO:O	9:M:767:HOH:O	2.12	0.67
1:M:422:LYS:NZ	1:M:574:ASP:OD2	2.29	0.66
1:M:438:ARG:O	1:M:441:ARG:HD3	1.97	0.65
1:E:351:MET:CE	1:E:352:TRP:CD1	2.81	0.64
1:M:382:ASP:OD1	9:M:787:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:284:ASN:HB2	1:I:575:TRP:CE2	2.35	0.60
1:M:250:THR:O	1:M:251:ASN:CB	2.49	0.60
1:M:284:ASN:HD22	1:M:284:ASN:N	1.99	0.60
1:M:318:GLU:O	8:M:607:CAC:AS	2.80	0.59
1:A:333:PRO:O	9:A:725:HOH:O	2.17	0.59
1:A:574:ASP:HB3	9:A:802:HOH:O	2.02	0.58
1:M:387:MET:CE	1:M:395:ILE:HD12	2.34	0.57
1:E:514:ARG:HD2	2:F:5:DG:OP2	2.04	0.57
1:M:291:LYS:HD3	1:M:292:PRO:O	2.05	0.57
2:B:1:DC:H2'	2:B:2:DG:C8	2.40	0.56
1:A:394:GLU:HG3	1:A:479:LEU:HD11	1.88	0.56
1:A:387:MET:HE2	1:A:391:GLU:HB3	1.89	0.53
1:M:438:ARG:O	1:M:441:ARG:CD	2.56	0.53
1:A:364:ARG:HG3	1:A:377:LEU:HD21	1.90	0.53
1:E:422:LYS:NZ	1:E:574:ASP:OD2	2.39	0.53
1:M:318:GLU:O	8:M:607:CAC:O2	2.27	0.53
1:A:308:ARG:O	1:A:312:LYS:HG3	2.10	0.52
1:A:361:GLU:N	1:A:361:GLU:CD	2.63	0.52
1:E:407:ASN:ND2	1:E:439:SER:OG	2.44	0.51
1:A:431:LEU:C	1:A:431:LEU:HD23	2.31	0.51
1:M:290:HIS:CD2	1:M:291:LYS:HB2	2.47	0.50
1:A:387:MET:CE	1:A:391:GLU:HG2	2.42	0.50
1:M:255:HIS:H	1:M:255:HIS:CD2	2.30	0.50
1:E:504:LEU:HD21	1:E:516:MET:HE1	1.92	0.50
1:I:314:ILE:HD12	1:I:315:GLU:N	2.27	0.50
1:M:557:LYS:HG3	9:M:776:HOH:O	2.12	0.50
1:E:558:ASP:OD1	1:E:561:ARG:NH2	2.45	0.49
1:M:357:PHE:O	1:M:358:ARG:NH1	2.37	0.49
1:E:538:ARG:HA	1:E:544:LYS:O	2.12	0.49
1:E:504:LEU:HD21	1:E:516:MET:CE	2.42	0.49
1:M:470:GLN:HG2	1:M:494:VAL:HG22	1.94	0.49
1:M:256:ILE:HD13	1:M:313:ILE:HG23	1.94	0.49
1:E:302:ILE:HB	1:E:305:ILE:HD12	1.95	0.49
1:A:330:GLU:O	1:A:333:PRO:HD2	2.13	0.49
1:A:387:MET:HE3	1:A:391:GLU:HG2	1.94	0.49
1:E:279:TYR:OH	1:E:312:LYS:HE3	2.13	0.48
1:I:400:GLN:HG3	1:I:412:CYS:HB2	1.95	0.48
1:A:387:MET:HE1	1:A:392:ALA:HA	1.95	0.47
1:I:407:ASN:ND2	1:I:439:SER:OG	2.47	0.47
1:I:436:ASP:C	1:I:436:ASP:OD1	2.53	0.47
1:A:265:LYS:HE3	1:A:336:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:9:DC:H2'	2:N:10:DT:H71	1.97	0.46
1:E:431:LEU:CD1	1:E:492:ILE:HG23	2.44	0.45
1:I:256:ILE:HD11	1:I:317:LEU:CD1	2.47	0.45
1:M:436:ASP:OD1	1:M:436:ASP:C	2.55	0.45
1:E:525:MET:CE	1:E:563:LEU:HD23	2.47	0.45
1:E:332:VAL:N	1:E:333:PRO:CD	2.80	0.45
1:A:579:HIS:CB	9:A:730:HOH:O	2.58	0.44
4:D:3:DC:H2"	4:D:4:DG:C8	2.52	0.44
1:I:515:SER:HB3	1:I:576:LEU:HD23	1.99	0.44
1:E:321:HIS:HB3	9:E:708:HOH:O	2.16	0.44
1:E:534:THR:O	1:E:536:VAL:HG23	2.18	0.44
1:I:291:LYS:HB2	1:I:292:PRO:HD2	1.99	0.44
1:M:538:ARG:HB3	1:M:538:ARG:CZ	2.47	0.44
1:A:267:TYR:CZ	1:A:275:ARG:HD3	2.52	0.44
1:A:360:LEU:O	1:A:363:ILE:HB	2.18	0.44
1:A:514:ARG:HD2	2:B:5:DG:OP2	2.18	0.43
1:I:569:GLU:O	1:I:570:PRO:C	2.57	0.43
2:F:1:DC:H2"	2:F:2:DG:H5'	1.99	0.43
1:A:514:ARG:HD3	2:B:5:DG:N7	2.34	0.43
1:M:387:MET:HE2	1:M:392:ALA:N	2.33	0.43
1:E:523:LYS:NZ	1:E:563:LEU:O	2.48	0.43
1:E:365:SER:OG	1:E:366:GLN:HG3	2.17	0.43
1:E:523:LYS:O	1:E:525:MET:HG3	2.18	0.42
1:M:541:HIS:ND1	1:M:541:HIS:O	2.52	0.42
1:I:431:LEU:HD23	1:I:503:LEU:HD13	2.01	0.42
1:A:274:TRP:CE3	1:A:274:TRP:HA	2.54	0.42
1:E:569:GLU:HG3	1:E:570:PRO:HD2	2.01	0.42
1:M:541:HIS:HA	1:M:543:CYS:SG	2.59	0.42
1:M:387:MET:HE2	1:M:391:GLU:HB3	2.01	0.42
1:E:451:LEU:HB3	1:E:457:LEU:HG	2.02	0.42
1:A:577:GLU:H	1:A:577:GLU:CD	2.23	0.42
1:I:286:LEU:HD11	1:I:313:ILE:HD11	2.00	0.41
2:F:9:DC:H5"	9:F:206:HOH:O	2.20	0.41
1:A:314:ILE:O	1:A:315:GLU:C	2.58	0.41
1:M:411:LEU:HD22	1:M:435:PRO:HD3	2.01	0.41
1:A:514:ARG:NH1	9:A:792:HOH:O	2.54	0.41
1:E:305:ILE:HG23	1:E:309:MET:HB3	2.01	0.41
1:E:519:LEU:HD23	1:E:519:LEU:C	2.41	0.41
1:A:387:MET:HE2	1:A:392:ALA:N	2.35	0.41
1:A:492:ILE:HG23	1:A:506:PHE:CZ	2.56	0.41
1:M:541:HIS:CG	1:M:541:HIS:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:MET:HE2	1:A:391:GLU:CB	2.50	0.40
1:M:351:MET:CE	1:M:352:TRP:CD1	3.04	0.40
1:A:290:HIS:CE1	9:A:763:HOH:O	2.74	0.40
1:A:529:GLU:OE2	9:A:784:HOH:O	2.22	0.40
1:A:535:ALA:HB3	1:A:548:GLY:CA	2.45	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	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

All (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
1	E	544	LYS
1	E	545	VAL
1	M	329	SER
1	M	544	LYS
1	E	463	SER

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Mol	Chain	Res	Type
1	M	290	HIS
1	A	536	VAL
1	M	545	VAL

### 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	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

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	361	GLU
1	A	378	LYS
1	A	506	PHE
1	A	569	GLU
1	A	576	LEU
1	A	577	GLU
1	E	254	LEU
1	E	314	ILE
1	E	384	LEU
1	E	397	GLN
1	E	401	LYS
1	E	404	GLN
1	E	408	SER
1	E	413	VAL
1	E	444	PHE
1	E	449	ASP
1	E	472	LYS
1	E	506	PHE

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Mol	Chain	Res	Type
1	E	514	ARG
1	E	532	LEU
1	E	534	THR
1	E	538	ARG
1	E	544	LYS
1	E	568	ARG
1	E	576	LEU
1	I	260	LEU
1	I	277	LEU
1	I	315	GLU
1	I	317	LEU
1	I	324	LYS
1	I	385	GLU
1	I	429	ASP
1	I	453	GLN
1	I	503	LEU
1	I	519	LEU
1	M	250	THR
1	M	284	ASN
1	M	286	LEU
1	M	302	ILE
1	M	314	ILE
1	M	317	LEU
1	M	368	SER
1	M	384	LEU
1	M	385	GLU
1	M	411	LEU
1	M	413	VAL
1	M	438	ARG
1	M	449	ASP
1	M	488	ARG
1	M	489	LEU
1	M	538	ARG
1	M	544	LYS
1	M	565	LEU
1	M	568	ARG
1	M	576	LEU
1	M	578	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	A	340	ASN
1	A	372	GLN
1	A	373	GLN
1	A	404	GLN
1	A	470	GLN
1	A	511	HIS
1	A	580	HIS
1	E	290	HIS
1	E	372	GLN
1	E	404	GLN
1	I	372	GLN
1	I	397	GLN
1	I	404	GLN
1	I	453	GLN
1	M	255	HIS
1	M	284	ASN
1	M	290	HIS
1	M	372	GLN
1	M	379	HIS
1	M	464	GLN
1	M	471	GLN
1	M	486	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 carbohydrates 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
7	ACT	M	601	-	1,3,3	0.78	0	0,3,3	0.00	-
7	ACT	F	102	-	1,3,3	2.42	1 (100%)	0,3,3	0.00	-
7	ACT	B	102	-	1,3,3	1.85	0	0,3,3	0.00	-
7	ACT	I	605	-	1,3,3	2.37	1 (100%)	0,3,3	0.00	-
5	1S0	M	602	6	23,29,29	0.76	0	30,45,45	1.26	3 (10%)
5	1S0	E	601	6	23,29,29	0.77	0	30,45,45	1.35	2 (6%)
5	1S0	A	601	6	23,29,29	1.07	2 (8%)	30,45,45	1.02	2 (6%)
8	CAC	M	607	-	0,4,4	0.00	-	0,6,6	0.00	-
5	1S0	I	601	6	23,29,29	0.62	0	30,45,45	1.45	2 (6%)

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	-	3/19/34/34	0/2/2/2
5	1S0	E	601	6	-	4/19/34/34	0/2/2/2
5	1S0	M	602	6	-	2/19/34/34	0/2/2/2
5	1S0	I	601	6	-	2/19/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	1S0	CAZ-NAR	-3.04	1.32	1.38
7	F	102	ACT	CH3-C	2.42	1.51	1.48
7	I	605	ACT	CH3-C	2.37	1.51	1.48
5	A	601	1S0	OAE-CAT	-2.06	1.39	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	601	1S0	CAZ-NAR-CBB	5.24	121.65	116.34
5	E	601	1S0	PAB-OAG-PAA	-2.87	122.99	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	602	1S0	CBA-CBB-NAR	-2.52	118.81	121.72
5	E	601	1S0	OAL-PAB-OAM	2.44	124.33	112.24
5	A	601	1S0	OAJ-PAA-OAI	2.42	124.19	112.24
5	A	601	1S0	OAP-PAC-OAO	2.25	119.50	110.68
5	M	602	1S0	OAL-PAB-OAM	2.20	123.11	112.24
5	M	602	1S0	OAP-PAC-OAK	-2.18	97.31	104.64
5	I	601	1S0	OAN-PAC-OAP	2.15	115.84	107.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	601	1S0	PAB-OAK-PAC-OAP
5	I	601	1S0	OAD-CAW-NAQ-CAY
5	M	602	1S0	OAD-CAW-NAQ-CAY
5	A	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
5	A	601	1S0	PAB-OAK-PAC-OAO
5	E	601	1S0	PAA-OAG-PAB-OAL
5	A	601	1S0	PAA-OAG-PAB-OAM
5	E	601	1S0	PAB-OAK-PAC-OAO

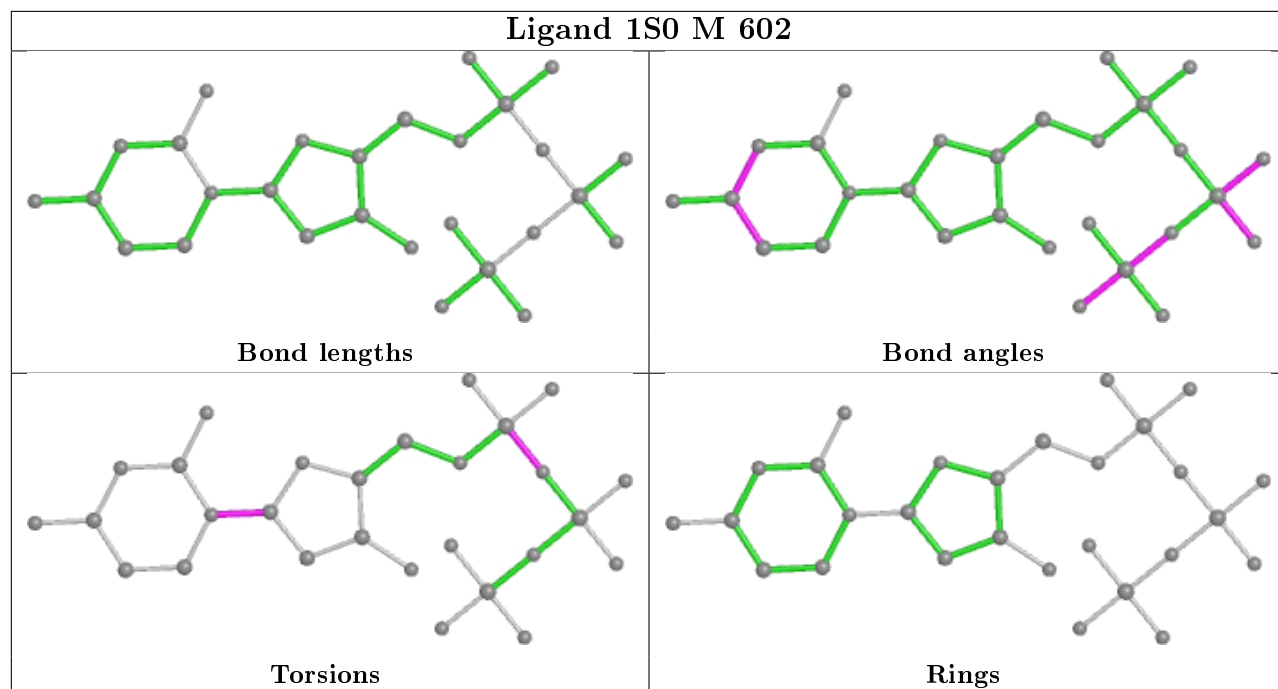
There are no ring outliers.

1 monomer is involved in 2 short contacts:

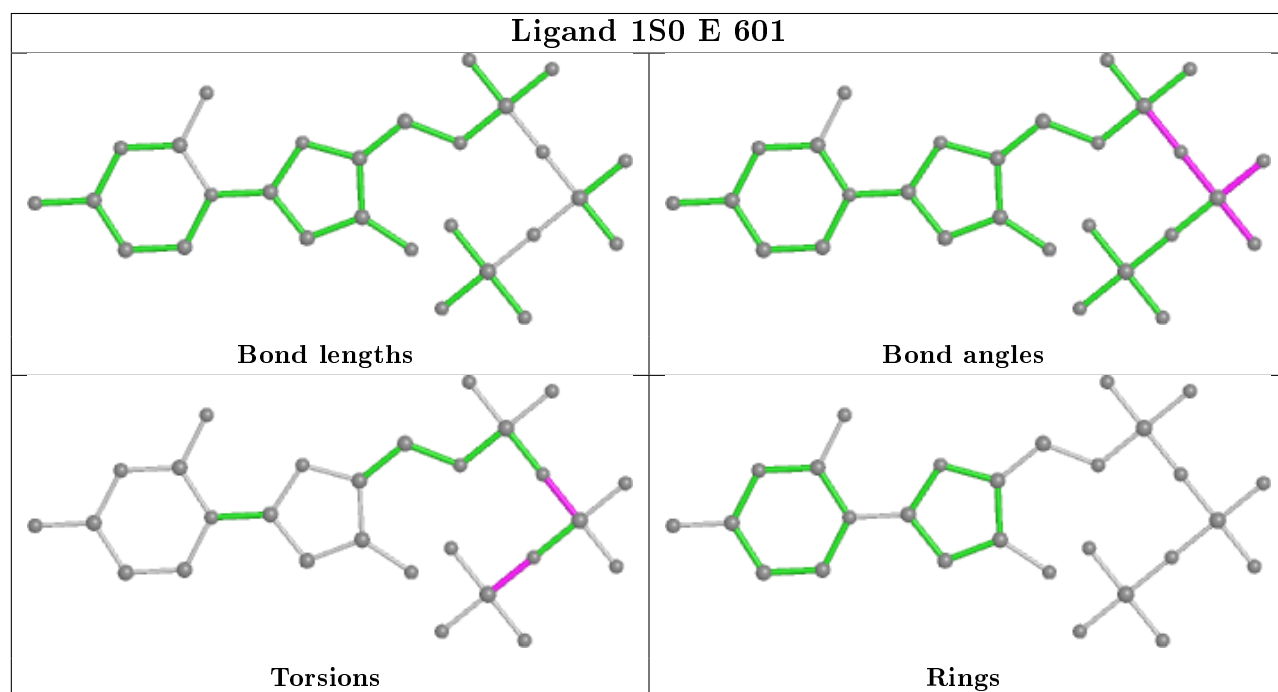
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	607	CAC	2	0

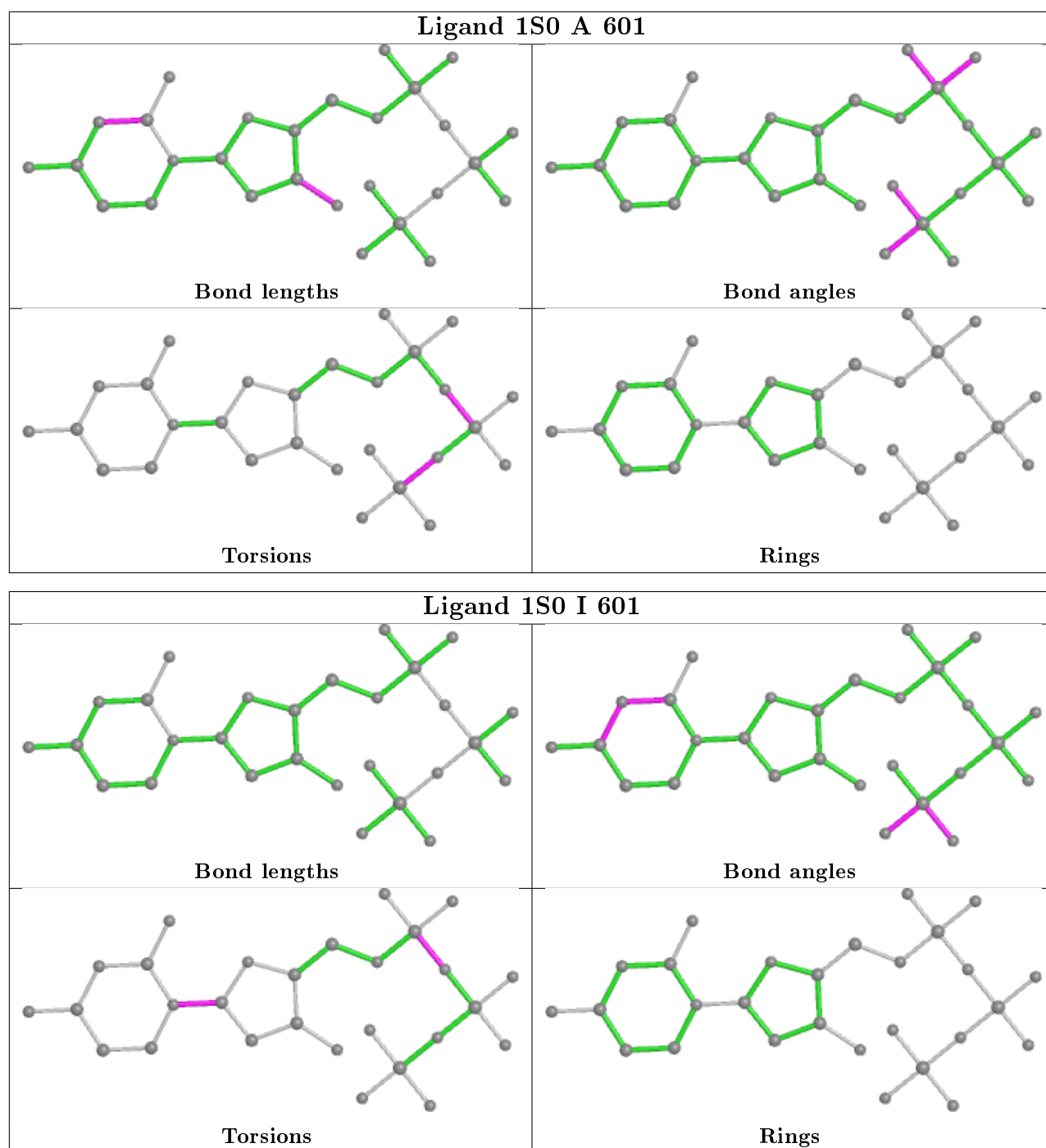
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 1S0 M 602



## Ligand 1S0 E 601





## 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<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	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

All (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

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Mol	Chain	Res	Type	RSRZ
1	M	250	THR	5.8
1	M	543	CYS	5.5
1	I	581	HIS	5.1
1	M	578	HIS	4.9
1	E	539	ASN	4.9
1	I	546	GLY	4.8
1	M	545	VAL	4.7
1	M	541	HIS	4.4
1	A	255	HIS	4.4
1	E	543	CYS	4.2
1	M	542	GLY	4.0
1	I	323	ARG	4.0
1	I	321	HIS	3.9
1	I	482	PRO	3.5
1	E	545	VAL	3.5
1	E	537	VAL	3.4
1	I	580	HIS	3.3
1	M	538	ARG	3.2
1	E	249	ALA	3.2
1	I	578	HIS	3.1
1	M	575	TRP	3.0
1	A	321	HIS	2.9
1	M	537	VAL	2.8
1	A	327	HIS	2.7
1	A	534	THR	2.7
1	I	250	THR	2.7
1	E	535	ALA	2.7
1	A	535	ALA	2.7
1	A	323	ARG	2.7
1	I	483	GLY	2.7
1	E	330	GLU	2.5
1	A	537	VAL	2.5
1	M	330	GLU	2.4
1	I	537	VAL	2.4
1	E	542	GLY	2.3
1	I	326	ASP	2.3
1	I	255	HIS	2.2
1	I	545	VAL	2.2
1	I	438	ARG	2.1
1	E	538	ARG	2.1
1	I	327	HIS	2.1
1	E	390	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	549	ARG	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 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.

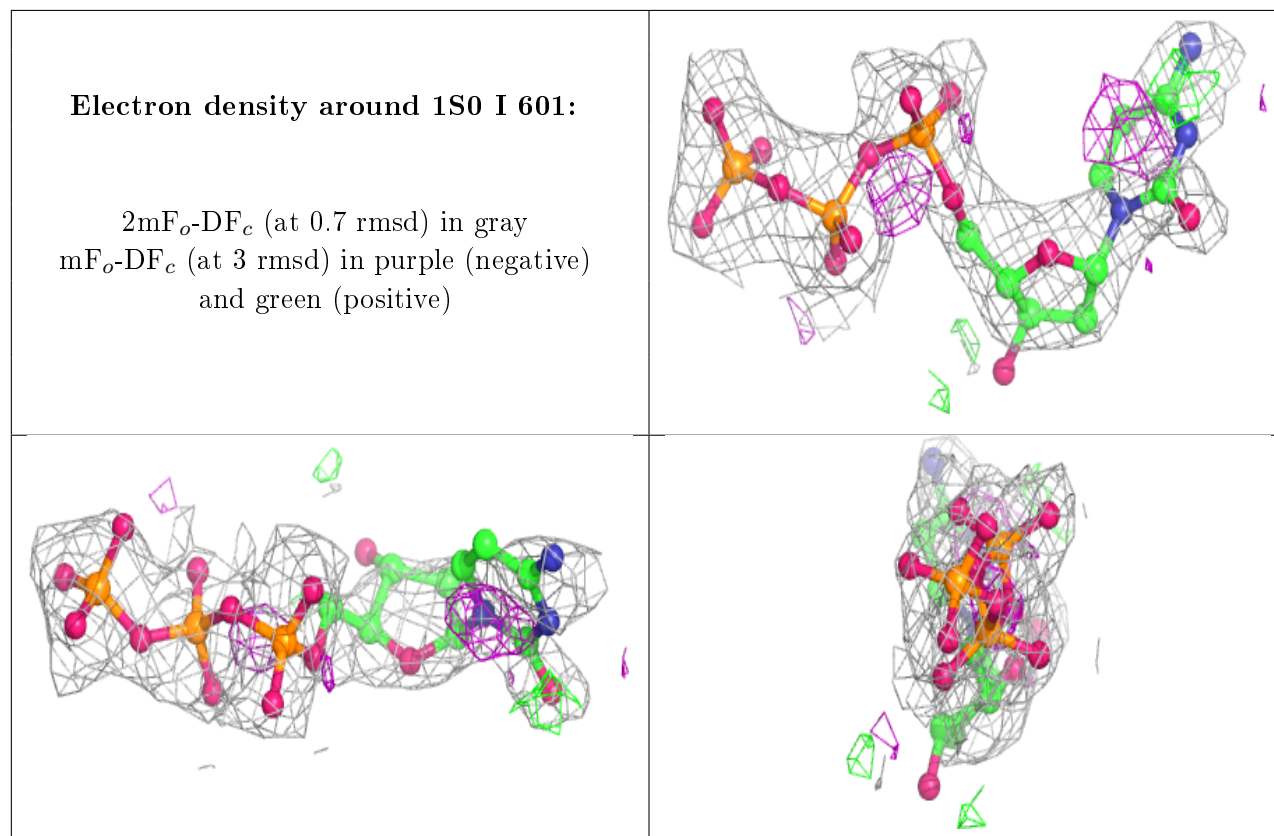
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	CA	J	102	1/1	0.48	0.15	81,81,81,81	0
6	CA	E	604	1/1	0.54	0.34	78,78,78,78	0
6	CA	E	605	1/1	0.72	0.11	56,56,56,56	0
6	CA	I	602	1/1	0.73	0.14	69,69,69,69	0
6	CA	M	604	1/1	0.73	0.13	72,72,72,72	0
6	CA	I	603	1/1	0.75	0.13	77,77,77,77	0
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	ISO	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
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
5	ISO	M	602	28/28	0.93	0.12	31,47,58,61	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	E	603	1/1	0.97	0.05	37,37,37,37	0
6	CA	E	606	1/1	0.97	0.19	41,41,41,41	0

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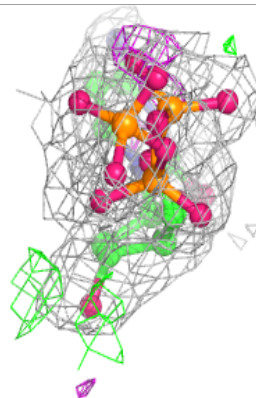
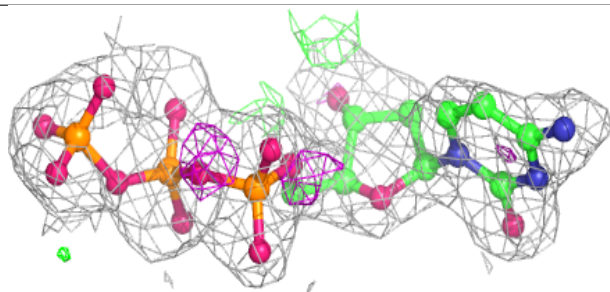
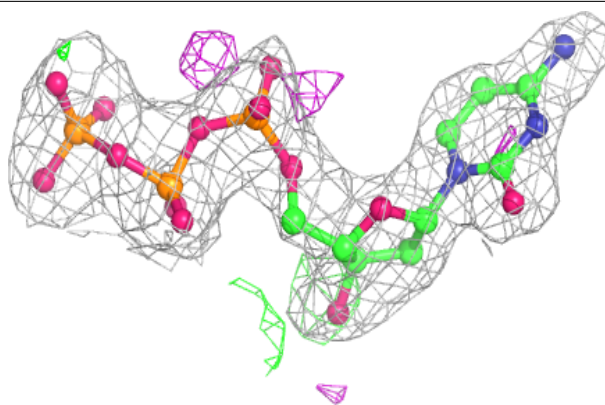
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	1S0	E	601	28/28	0.97	0.11	23,30,39,43	0
6	CA	A	604	1/1	0.97	0.17	34,34,34,34	0
6	CA	L	101	1/1	0.97	0.10	78,78,78,78	0
6	CA	E	602	1/1	0.98	0.07	34,34,34,34	0
6	CA	I	604	1/1	0.98	0.09	20,20,20,20	1
6	CA	A	603	1/1	0.98	0.09	20,20,20,20	0
6	CA	A	602	1/1	0.99	0.10	20,20,20,20	0
6	CA	A	606	1/1	0.99	0.05	42,42,42,42	0
5	1S0	A	601	28/28	0.99	0.13	14,18,21,23	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.

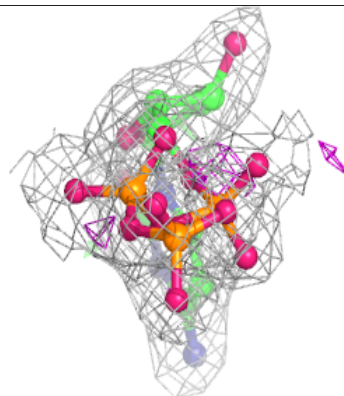
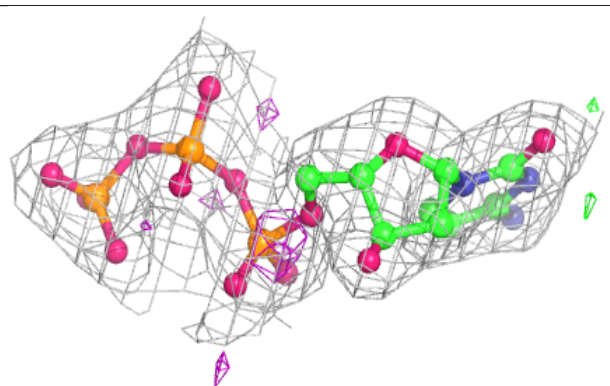
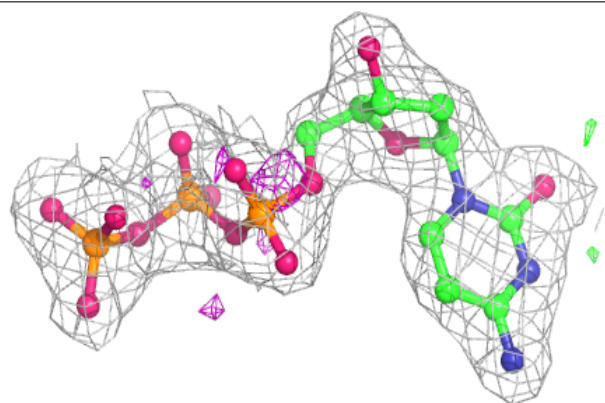


**Electron density around 1S0 M 602:**

$2mF_o - DF_c$  (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:**

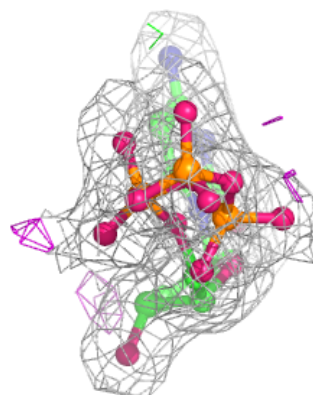
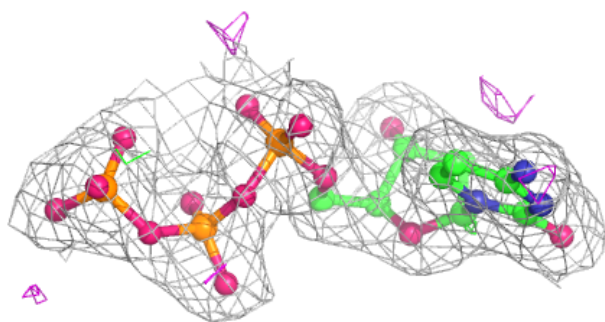
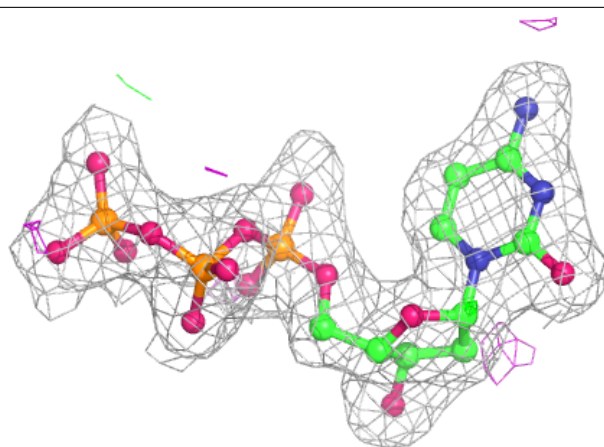
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**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 [i](#)

There are no such residues in this entry.