



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:44 pm BST

PDB ID : 4K4I  
Title : Ternary crystal structures of a human DNA POLYMERASE LAMBDA IN COMPLEX WITH DNA AND (-)FTC-TP.  
Authors : Vyas, R.; Suo, Z.  
Deposited on : 2013-04-12  
Resolution : 2.25 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

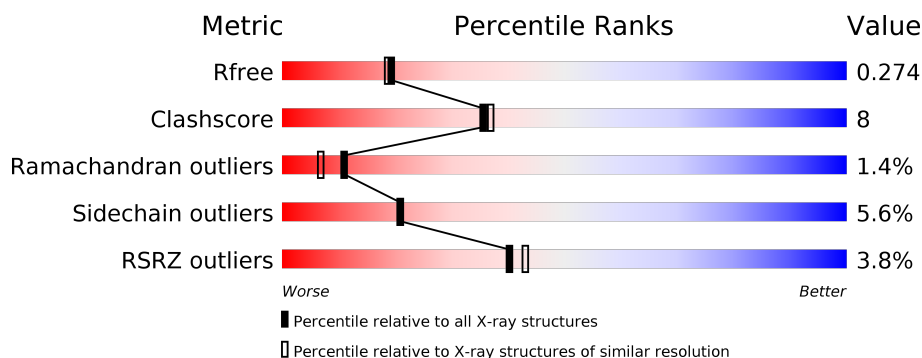
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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>5%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• • •</div> </div> </div>
1	E	340	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• •</div> </div> </div>
1	I	340	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	M	340	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• •</div> </div> </div>
2	B	11	<div> <div></div> <div> <div>73%</div> <div>27%</div> </div> </div>
2	F	11	<div> <div></div> <div> <div>73%</div> <div>9%</div> <div>18%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	J	11	 91% 9%
2	N	11	 73% 27%
3	C	6	 100%
3	G	6	 100%
3	K	6	 83% 17%
3	O	6	 83% 17%
4	D	4	 25% 25% 50%
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 12760 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	333	Total	C	N	O	S	0	3	0
			2649	1663	489	485	12			
1	E	329	Total	C	N	O	S	0	0	0
			2589	1626	474	477	12			
1	I	325	Total	C	N	O	S	0	0	0
			2574	1617	473	473	11			
1	M	329	Total	C	N	O	S	0	1	0
			2592	1628	474	478	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			

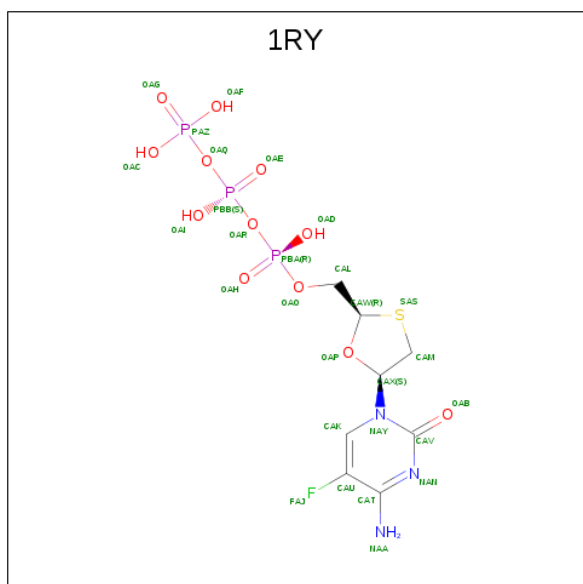
- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*AP\*GP\*TP\*AP\*C)-3').

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 [[(2R,5S)-5-(4-azanyl-5-fluoranyl-2-oxidanylidene-pyrimidin-1-yl)-1,3-oxathiolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (three-letter code: 1RY) (formula: C<sub>8</sub>H<sub>13</sub>FN<sub>3</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total 28	C 8	F 1	N 3	O 12	P 3	S 1	0	0
5	E	1	Total 28	C 8	F 1	N 3	O 12	P 3	S 1	0	0
5	I	1	Total 28	C 8	F 1	N 3	O 12	P 3	S 1	0	0
5	M	1	Total 28	C 8	F 1	N 3	O 12	P 3	S 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	1	Total 1	Ca 1	0	0
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	6	Total 6	Ca 6	0	0
6	N	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:  $C_2H_3O_2$ ).



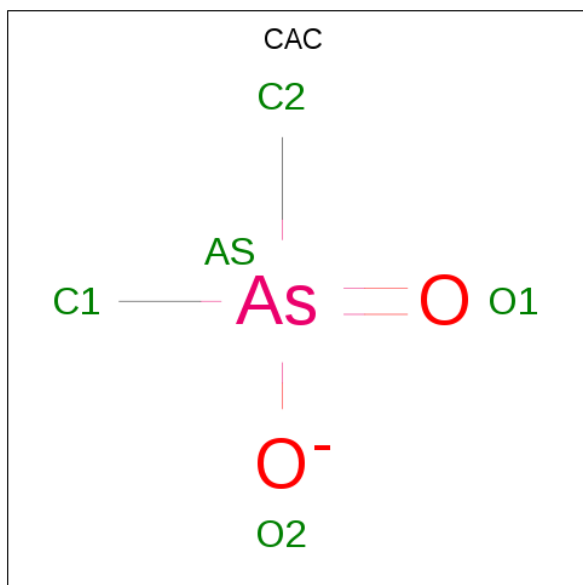
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0
7	B	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	As	C	O	0	0
			5	1	2	2		
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	129	Total	O	0	0
			129	129		
9	B	20	Total	O	0	0
			20	20		
9	C	13	Total	O	0	0
			13	13		
9	E	78	Total	O	0	0
			78	78		

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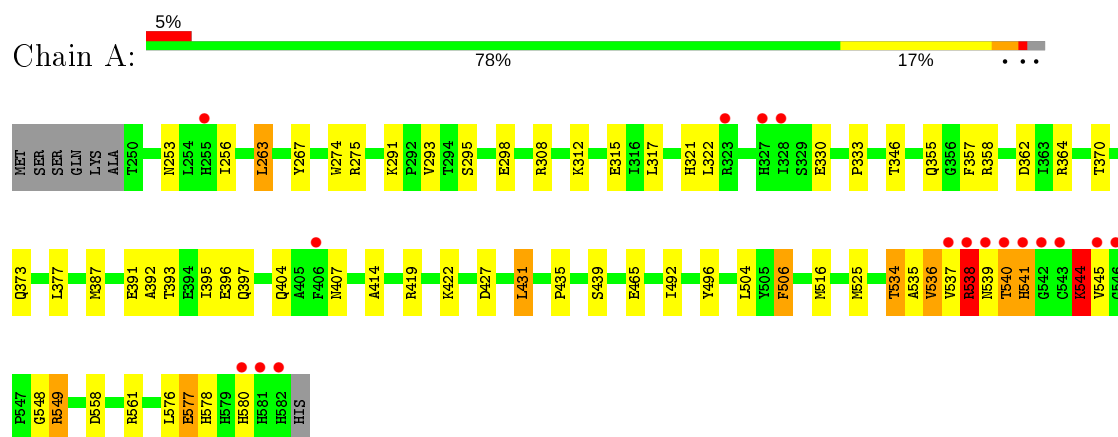
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	9	Total 9	O 9	0	0
9	G	2	Total 2	O 2	0	0
9	H	2	Total 2	O 2	0	0
9	I	76	Total 76	O 76	0	0
9	J	4	Total 4	O 4	0	0
9	K	9	Total 9	O 9	0	0
9	M	124	Total 124	O 124	0	0
9	N	8	Total 8	O 8	0	0
9	O	3	Total 3	O 3	0	0
9	P	2	Total 2	O 2	0	0

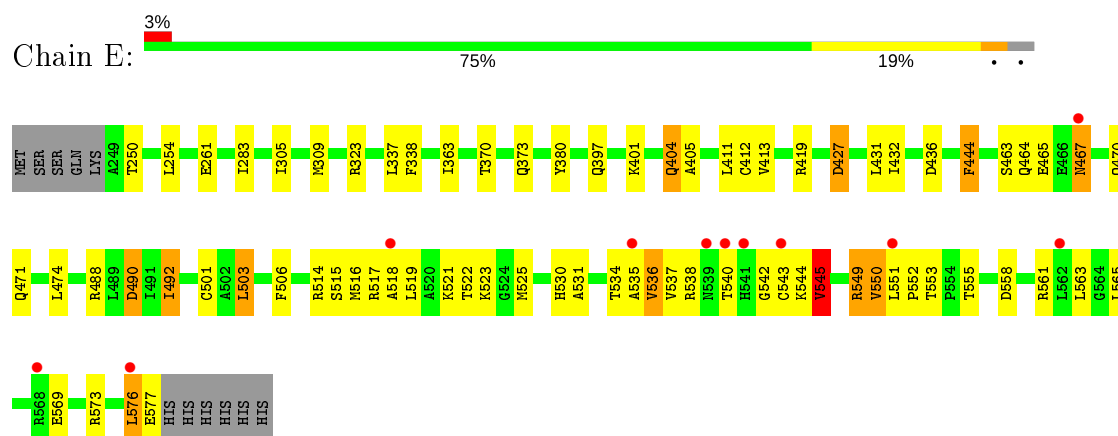
### 3 Residue-property plots [i](#)

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.

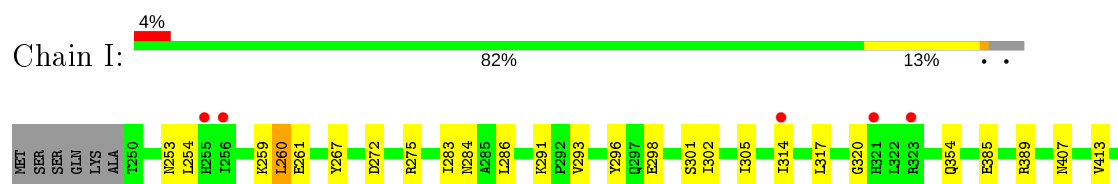
- Molecule 1: DNA polymerase lambda



- Molecule 1: DNA polymerase lambda

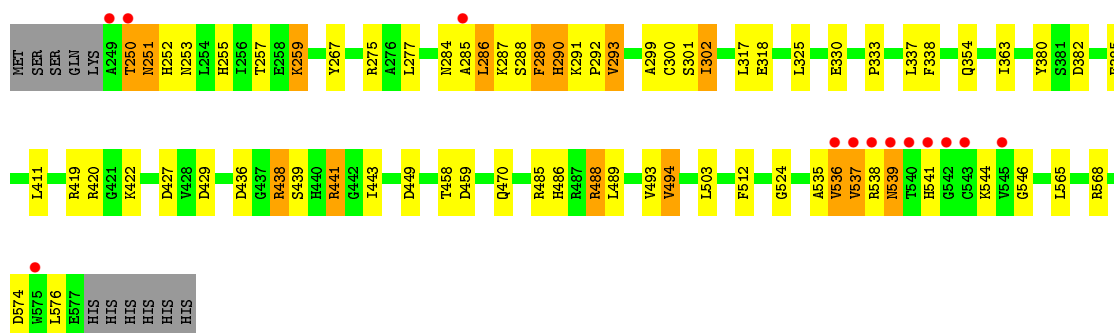
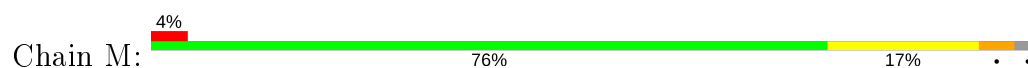


- Molecule 1: DNA polymerase lambda





- Molecule 1: DNA polymerase lambda



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



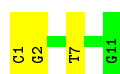
- Molecule 2: DNA (5'-D(\*CP\*GP\*GP\*CP\*GP\*GP\*TP\*AP\*CP\*TP\*G)-3')



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



- 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')

Chain G:  100%


There are no outlier residues recorded for this chain.

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

Chain K:  83% 17%




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

Chain O:  83% 17%



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

Chain D:  25% 25% 50%



- 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, $\alpha$ , $\beta$ , $\gamma$	194.44Å 97.58Å 105.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.03 – 2.25 45.03 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.03-2.25) 100.0 (45.03-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.212 , 0.274 0.216 , 0.274	Depositor DCC
$R_{free}$ test set	4788 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.6	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	0.93	EDS
Total number of atoms	12760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, 1RY, 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	0.85	1/2716 (0.0%)	0.94	4/3666 (0.1%)
1	E	0.76	0/2642	0.88	5/3566 (0.1%)
1	I	0.74	1/2628 (0.0%)	0.89	6/3546 (0.2%)
1	M	0.85	2/2648 (0.1%)	1.04	11/3574 (0.3%)
2	B	0.68	0/252	1.09	1/388 (0.3%)
2	F	0.51	0/252	1.01	3/388 (0.8%)
2	J	0.64	0/252	0.89	0/388
2	N	0.65	0/252	0.96	0/388
3	C	0.86	0/133	1.04	0/203
3	G	0.60	0/133	0.93	0/203
3	K	0.60	0/133	1.08	2/203 (1.0%)
3	O	0.73	0/133	0.98	1/203 (0.5%)
4	D	1.17	1/92 (1.1%)	1.11	2/138 (1.4%)
4	H	1.33	1/92 (1.1%)	0.88	0/138
4	L	1.08	1/92 (1.1%)	0.81	0/138
4	P	1.23	1/92 (1.1%)	0.84	0/138
All	All	0.80	8/12542 (0.1%)	0.95	35/17268 (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	M	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	DG	OP3-P	-10.91	1.48	1.61
4	P	1	DG	OP3-P	-10.16	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	DG	OP3-P	-9.65	1.49	1.61
4	L	1	DG	OP3-P	-8.95	1.50	1.61
1	M	429	ASP	CB-CG	6.77	1.66	1.51
1	M	427	ASP	CB-CG	5.74	1.63	1.51
1	I	429	ASP	CB-CG	5.50	1.63	1.51
1	A	465	GLU	CD-OE2	5.08	1.31	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	488	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	M	427	ASP	CB-CG-OD1	10.82	128.04	118.30
1	M	488	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	A	427	ASP	CB-CG-OD1	9.96	127.27	118.30
1	M	441	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	I	429	ASP	CB-CG-OD1	8.68	126.12	118.30
1	I	427	ASP	CB-CG-OD1	8.07	125.56	118.30
1	M	429	ASP	CB-CG-OD2	7.97	125.47	118.30
1	I	419	ARG	NE-CZ-NH2	-7.84	116.38	120.30
4	D	3	DC	O5'-P-OP2	-7.21	99.21	105.70
1	I	419	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	M	420	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	419	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	I	503	LEU	CA-CB-CG	6.43	130.08	115.30
2	F	4	DC	C1'-O4'-C4'	-6.36	103.74	110.10
2	B	9	DC	O5'-P-OP1	-6.33	100.01	105.70
4	D	3	DC	O5'-P-OP1	6.29	118.25	110.70
2	F	9	DC	O5'-P-OP1	5.95	117.84	110.70
1	M	420	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	419	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	488	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	M	485	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	E	427	ASP	CB-CG-OD2	5.51	123.26	118.30
3	K	1	DC	C5'-C4'-C3'	5.51	124.01	114.10
1	M	419	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	M	441	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	E	490	ASP	CB-CG-OD2	5.42	123.18	118.30
1	E	490	ASP	CB-CG-OD1	-5.33	113.50	118.30
3	K	1	DC	C5'-C4'-O4'	5.21	119.20	109.30
2	F	9	DC	O5'-P-OP2	-5.21	101.02	105.70
3	O	4	DT	O5'-P-OP1	-5.21	101.01	105.70
1	I	420	ARG	NE-CZ-NH1	5.18	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	517	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	M	459	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	358	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	2649	0	2639	54	0
1	E	2589	0	2590	58	0
1	I	2574	0	2566	23	0
1	M	2592	0	2595	52	0
2	B	225	0	125	1	0
2	F	225	0	125	4	0
2	J	225	0	125	1	0
2	N	225	0	125	2	0
3	C	119	0	68	0	0
3	G	119	0	69	0	0
3	K	119	0	69	0	0
3	O	119	0	69	0	0
4	D	83	0	45	2	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	11	0	0
5	E	28	0	11	0	0
5	I	28	0	11	0	0
5	M	28	0	12	1	0
6	A	6	0	0	0	0
6	B	1	0	0	0	0
6	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1	0	0	0	0
6	I	3	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	M	4	0	0	0	0
6	N	1	0	0	0	0
7	A	4	0	3	0	0
7	B	4	0	3	0	0
7	E	4	0	3	1	0
7	F	4	0	3	0	0
7	I	4	0	3	0	0
7	M	4	0	3	0	0
8	E	5	0	0	0	0
8	M	5	0	0	3	0
9	A	129	0	0	12	0
9	B	20	0	0	0	0
9	C	13	0	0	0	0
9	E	78	0	0	7	0
9	F	9	0	0	0	0
9	G	2	0	0	0	0
9	H	2	0	0	0	0
9	I	76	0	0	1	0
9	J	4	0	0	1	0
9	K	9	0	0	0	0
9	M	124	0	0	3	0
9	N	8	0	0	1	0
9	O	3	0	0	0	0
9	P	2	0	0	0	0
All	All	12760	0	11408	192	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 8.

All (192) 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:397:GLN:HG3	9:E:770:HOH:O	1.58	1.01
1:M:535:ALA:HB1	1:M:536:VAL:HG23	1.38	1.01
1:M:536:VAL:H	1:M:537:VAL:HA	1.23	1.01
1:E:521:LYS:NZ	2:F:4:DC:OP1	2.03	0.90
1:E:501:CYS:SG	1:E:531:ALA:HA	2.15	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:537:VAL:HG23	1:M:546:GLY:O	1.74	0.86
1:M:536:VAL:H	1:M:537:VAL:CA	1.89	0.84
1:E:444:PHE:CD2	1:E:465:GLU:OE1	2.32	0.83
1:A:396:GLU:HG3	1:A:414:ALA:HB2	1.61	0.82
1:A:333:PRO:O	9:A:722:HOH:O	2.00	0.80
1:I:253:ASN:HD21	1:I:293:VAL:H	1.28	0.79
1:E:551:LEU:O	1:E:553:THR:HG23	1.86	0.75
1:M:535:ALA:CB	1:M:536:VAL:HG23	2.16	0.74
1:I:298:GLU:O	1:I:301:SER:HB3	1.87	0.74
1:M:288:SER:O	1:M:289:PHE:HB2	1.87	0.73
8:M:606:CAC:O2	9:M:812:HOH:O	2.08	0.72
1:A:253:ASN:HD21	1:A:293:VAL:H	1.37	0.71
2:J:2:DG:OP2	9:J:204:HOH:O	2.07	0.71
1:I:259:LYS:NZ	1:I:320:GLY:O	2.26	0.68
1:M:318:GLU:O	8:M:606:CAC:AS	2.71	0.68
1:M:289:PHE:O	1:M:291:LYS:N	2.27	0.67
1:A:315:GLU:HG2	9:A:818:HOH:O	1.96	0.66
1:A:322:LEU:HA	9:A:818:HOH:O	1.95	0.66
1:M:535:ALA:HB1	1:M:536:VAL:CG2	2.22	0.66
1:M:252:HIS:ND1	9:M:735:HOH:O	2.28	0.66
2:N:7:DT:OP2	9:N:205:HOH:O	2.13	0.66
1:A:315:GLU:CG	9:A:818:HOH:O	2.43	0.65
1:E:261:GLU:HG3	1:E:283:ILE:HD13	1.79	0.65
1:M:422:LYS:NZ	1:M:574:ASP:OD2	2.31	0.63
1:A:312:LYS:NZ	4:D:1:DG:OP3	2.28	0.63
1:A:535:ALA:HA	1:A:548:GLY:HA3	1.81	0.62
1:A:431:LEU:C	1:A:431:LEU:HD23	2.20	0.61
1:M:535:ALA:HA	1:M:536:VAL:HG22	1.83	0.61
1:M:538:ARG:O	1:M:539:ASN:HB3	2.00	0.61
1:A:537:VAL:O	1:A:538:ARG:HB2	2.01	0.60
1:E:467:ASN:ND2	1:E:470:GLN:O	2.35	0.60
1:M:267:TYR:CZ	1:M:275:ARG:HD3	2.37	0.60
1:E:305:ILE:HG23	1:E:309:MET:HB3	1.82	0.59
1:E:543:CYS:SG	1:I:540:THR:HA	2.43	0.59
1:E:516:MET:N	9:E:760:HOH:O	2.35	0.59
1:I:436:ASP:OD2	1:I:439:SER:HB2	2.03	0.58
1:E:550:VAL:O	1:E:551:LEU:HG	2.04	0.58
1:M:338:PHE:CZ	1:M:363:ILE:HD11	2.39	0.58
1:E:431:LEU:HD12	1:E:492:ILE:HG23	1.85	0.57
2:B:1:DC:H2'	2:B:2:DG:C8	2.40	0.57
1:A:355:GLN:HA	1:E:552:PRO:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:MET:CE	1:A:395:ILE:HD12	2.35	0.56
1:A:321:HIS:O	9:A:818:HOH:O	2.18	0.56
1:A:387:MET:HE2	1:A:392:ALA:N	2.21	0.56
1:A:387:MET:HE1	1:A:392:ALA:HA	1.86	0.56
1:A:541:HIS:O	1:A:541:HIS:CG	2.59	0.56
1:E:576:LEU:HD12	9:E:760:HOH:O	2.06	0.55
1:A:357:PHE:CD1	1:A:362:ASP:HB3	2.42	0.55
1:E:551:LEU:O	1:E:552:PRO:C	2.43	0.55
1:I:272:ASP:OD2	1:I:275:ARG:NH1	2.38	0.55
1:M:337:LEU:HD12	1:M:380:TYR:OH	2.06	0.55
1:M:536:VAL:N	1:M:537:VAL:CA	2.66	0.55
1:E:463:SER:HB3	9:E:776:HOH:O	2.06	0.55
1:E:535:ALA:O	1:E:536:VAL:HG22	2.06	0.55
1:E:515:SER:C	9:E:760:HOH:O	2.44	0.55
1:M:277:LEU:HD12	1:M:277:LEU:O	2.07	0.55
1:M:512:PHE:CE1	1:M:576:LEU:HD13	2.42	0.55
1:E:323:ARG:CZ	1:E:323:ARG:HB3	2.37	0.54
1:E:538:ARG:HA	1:E:544:LYS:HA	1.89	0.54
1:I:260:LEU:HB3	1:I:283:ILE:HD11	1.90	0.53
1:M:438:ARG:O	1:M:441:ARG:HD3	2.08	0.53
1:M:470:GLN:HG2	1:M:494:VAL:HG22	1.91	0.53
1:E:338:PHE:CZ	1:E:363:ILE:HD11	2.43	0.53
1:I:296:TYR:HB2	1:I:314:ILE:HG21	1.90	0.53
1:A:577:GLU:H	1:A:577:GLU:CD	2.12	0.53
1:E:419:ARG:NH1	1:E:503:LEU:HD22	2.24	0.53
1:I:522:THR:HG23	9:I:755:HOH:O	2.09	0.53
1:E:544:LYS:O	1:E:545:VAL:HG13	2.07	0.53
1:M:535:ALA:CB	1:M:536:VAL:CG2	2.84	0.53
1:M:436:ASP:OD2	1:M:439:SER:OG	2.25	0.52
1:E:525:MET:CE	1:E:563:LEU:HD23	2.39	0.52
1:A:544:LYS:HD2	1:A:545:VAL:O	2.09	0.52
1:M:285:ALA:O	1:M:288:SER:O	2.28	0.52
1:E:555:THR:HA	7:E:608:ACT:H1	1.92	0.52
1:M:318:GLU:O	8:M:606:CAC:O1	2.27	0.52
1:M:438:ARG:NH1	1:M:438:ARG:HB3	2.25	0.52
1:M:252:HIS:CE1	9:M:735:HOH:O	2.63	0.52
1:A:536:VAL:N	9:A:817:HOH:O	2.42	0.51
1:A:548:GLY:O	1:A:549:ARG:CB	2.55	0.51
1:E:576:LEU:C	1:E:577:GLU:HG3	2.30	0.51
1:E:540:THR:HG23	1:E:540:THR:O	2.10	0.51
1:E:540:THR:HG23	1:E:543:CYS:SG	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:535:ALA:HA	1:M:536:VAL:CG2	2.41	0.50
1:I:413:VAL:HG21	1:I:503:LEU:HD11	1.93	0.50
1:M:289:PHE:C	1:M:291:LYS:H	2.14	0.50
1:A:330:GLU:HA	9:A:806:HOH:O	2.11	0.50
1:M:536:VAL:N	1:M:537:VAL:HA	2.07	0.50
1:M:288:SER:O	1:M:289:PHE:CB	2.55	0.49
1:A:387:MET:HE1	1:A:395:ILE:HD12	1.92	0.49
1:M:267:TYR:CE2	1:M:275:ARG:HD3	2.48	0.49
1:M:538:ARG:O	1:M:539:ASN:CB	2.60	0.49
1:I:431:LEU:HD23	1:I:503:LEU:HD13	1.94	0.49
1:M:338:PHE:CE1	1:M:363:ILE:HD11	2.48	0.49
1:E:411:LEU:O	1:E:432:ILE:HA	2.13	0.48
1:E:431:LEU:CD1	1:E:492:ILE:HG23	2.44	0.48
1:E:523:LYS:O	1:E:525:MET:HG3	2.13	0.48
1:M:535:ALA:CA	1:M:536:VAL:CG2	2.91	0.48
1:I:302:ILE:HB	1:I:305:ILE:HD12	1.95	0.48
1:A:504:LEU:HD21	1:A:516:MET:CE	2.43	0.48
1:A:558:ASP:OD1	1:A:561:ARG:NH2	2.44	0.48
1:A:535:ALA:C	9:A:817:HOH:O	2.52	0.47
1:M:253:ASN:O	1:M:257:THR:HG23	2.14	0.47
1:A:346:THR:HG23	9:A:745:HOH:O	2.13	0.47
1:E:467:ASN:CG	1:E:467:ASN:O	2.52	0.47
1:A:548:GLY:O	1:A:549:ARG:HB3	2.14	0.47
1:E:427:ASP:C	1:E:427:ASP:OD1	2.53	0.47
1:I:576:LEU:O	1:I:580:HIS:HB2	2.15	0.47
1:A:541:HIS:O	1:A:541:HIS:CD2	2.68	0.46
1:I:385:GLU:OE1	1:I:485:ARG:CZ	2.63	0.46
1:I:284:ASN:HB2	1:I:575:TRP:CE2	2.51	0.46
1:A:535:ALA:CA	9:A:817:HOH:O	2.63	0.46
1:A:308:ARG:O	1:A:312:LYS:HG3	2.15	0.46
1:E:370:THR:OG1	1:E:373:GLN:HG3	2.15	0.46
1:E:492:ILE:HD13	1:E:506:PHE:CZ	2.50	0.46
1:A:387:MET:HE3	1:A:391:GLU:HG2	1.96	0.46
1:M:250:THR:O	1:M:251:ASN:CB	2.64	0.46
1:E:518:ALA:O	1:E:522:THR:HG23	2.16	0.46
1:M:255:HIS:H	1:M:255:HIS:CD2	2.34	0.45
1:M:252:HIS:O	1:M:292:PRO:HB3	2.16	0.45
1:A:355:GLN:HE21	1:A:357:PHE:HE2	1.63	0.45
1:E:519:LEU:HD23	1:E:519:LEU:C	2.36	0.45
1:A:387:MET:HE2	1:A:391:GLU:HB3	1.99	0.45
1:A:535:ALA:HA	9:A:817:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:GLN:HE21	1:E:404:GLN:HA	1.82	0.45
1:A:357:PHE:HB3	1:A:362:ASP:HB2	1.99	0.45
1:I:413:VAL:HG21	1:I:503:LEU:CD1	2.47	0.45
1:A:263:LEU:CD1	1:A:267:TYR:CE2	3.00	0.44
1:A:291:LYS:NZ	1:A:298:GLU:OE2	2.37	0.44
1:A:274:TRP:HA	1:A:274:TRP:CE3	2.52	0.44
1:I:261:GLU:HG3	1:I:283:ILE:HD13	2.00	0.44
1:M:438:ARG:CZ	1:M:438:ARG:HB3	2.47	0.44
1:A:263:LEU:CD1	1:A:267:TYR:HE2	2.31	0.44
1:A:404:GLN:NE2	9:A:824:HOH:O	2.34	0.44
1:E:519:LEU:HD13	1:E:565:LEU:HD11	1.99	0.44
1:E:569:GLU:HG3	9:E:710:HOH:O	2.18	0.44
2:N:1:DC:H2"	2:N:2:DG:C8	2.52	0.44
1:A:267:TYR:CZ	1:A:275:ARG:HD3	2.53	0.44
1:I:298:GLU:O	1:I:301:SER:CB	2.62	0.44
1:E:569:GLU:O	1:E:573:ARG:HG3	2.18	0.44
1:A:539:ASN:O	1:A:540:THR:C	2.55	0.43
1:E:543:CYS:SG	1:I:540:THR:HB	2.57	0.43
1:E:467:ASN:O	1:E:530:HIS:CE1	2.71	0.43
1:M:470:GLN:CG	1:M:494:VAL:HG22	2.47	0.43
5:M:601:1RY:OAI	5:M:601:1RY:OAG	2.30	0.43
1:A:435:PRO:HA	1:A:496:TYR:CD1	2.53	0.43
1:E:337:LEU:HD12	1:E:380:TYR:OH	2.19	0.43
1:E:543:CYS:O	1:E:544:LYS:HB2	2.19	0.43
1:E:444:PHE:CD2	1:E:471:GLN:HB3	2.53	0.43
1:I:291:LYS:HE3	1:I:298:GLU:OE2	2.19	0.43
1:M:286:LEU:O	1:M:287:LYS:C	2.57	0.43
4:D:3:DC:H2"	4:D:4:DG:C8	2.54	0.43
1:E:465:GLU:HA	1:E:471:GLN:HB3	2.00	0.43
1:M:293:VAL:HG21	1:M:299:ALA:HB2	2.00	0.42
1:E:525:MET:HE1	1:E:563:LEU:HD23	2.01	0.42
2:F:8:DA:H2"	2:F:9:DC:OP2	2.19	0.42
1:A:492:ILE:HG12	1:A:506:PHE:CZ	2.54	0.42
1:A:544:LYS:CG	1:A:545:VAL:N	2.81	0.42
1:E:250:THR:HA	9:E:715:HOH:O	2.19	0.42
1:E:412:CYS:SG	1:E:432:ILE:HG12	2.59	0.42
1:E:464:GLN:O	1:E:471:GLN:HA	2.19	0.42
1:E:474:LEU:HD22	1:E:490:ASP:OD1	2.19	0.42
1:A:253:ASN:HD22	1:A:256:ILE:HD12	1.83	0.42
1:E:464:GLN:OE1	2:F:8:DA:H4'	2.18	0.42
1:A:393:THR:O	1:A:397:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:524:GLY:O	1:M:535:ALA:HB2	2.20	0.42
1:E:525:MET:O	1:E:538:ARG:NH2	2.52	0.42
1:E:444:PHE:CD2	1:E:471:GLN:CB	3.02	0.42
1:I:286:LEU:HG	1:I:305:ILE:HD11	2.02	0.42
1:M:286:LEU:HA	1:M:286:LEU:HD12	1.95	0.41
1:M:300:CYS:C	1:M:302:ILE:H	2.23	0.41
1:A:578:HIS:CD2	1:A:580:HIS:CE1	3.09	0.41
1:M:284:ASN:O	1:M:285:ALA:C	2.56	0.41
1:M:382:ASP:HB3	1:M:486:HIS:O	2.21	0.41
1:A:407:ASN:C	1:A:407:ASN:OD1	2.58	0.41
1:M:289:PHE:C	1:M:291:LYS:N	2.72	0.41
1:E:538:ARG:O	1:E:542:GLY:HA2	2.21	0.41
1:A:370:THR:H	1:A:373:GLN:NE2	2.18	0.41
1:E:576:LEU:C	1:E:577:GLU:CG	2.88	0.41
1:A:431:LEU:C	1:A:431:LEU:CD2	2.89	0.41
1:M:259:LYS:HB3	1:M:325:LEU:HD11	2.03	0.41
1:M:330:GLU:O	1:M:333:PRO:HD2	2.21	0.40
1:A:525:MET:HG2	1:A:534:THR:HA	2.03	0.40
1:E:464:GLN:HB3	2:F:8:DA:O3'	2.22	0.40
1:M:443:ILE:HD13	1:M:443:ILE:HA	1.91	0.40
1:A:364:ARG:HG3	1:A:377:LEU:HD21	2.03	0.40
1:I:267:TYR:CZ	1:I:275:ARG:HD3	2.57	0.40
1:I:536:VAL:HG21	1:I:539:ASN:OD1	2.22	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	334/340 (98%)	313 (94%)	17 (5%)	4 (1%)	13 9
1	E	327/340 (96%)	296 (90%)	25 (8%)	6 (2%)	8 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	321/340 (94%)	308 (96%)	12 (4%)	1 (0%)	41	46
1	M	328/340 (96%)	306 (93%)	15 (5%)	7 (2%)	7	3
All	All	1310/1360 (96%)	1223 (93%)	69 (5%)	18 (1%)	11	7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	ARG
1	M	251	ASN
1	M	289	PHE
1	M	290	HIS
1	M	536	VAL
1	M	537	VAL
1	M	539	ASN
1	A	540	THR
1	E	537	VAL
1	E	545	VAL
1	E	549	ARG
1	E	550	VAL
1	E	558	ASP
1	E	405	ALA
1	M	301	SER
1	A	544	LYS
1	A	549	ARG
1	I	407	ASN

### 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	284/287 (99%)	270 (95%)	14 (5%)	25	27
1	E	276/287 (96%)	260 (94%)	16 (6%)	20	20
1	I	275/287 (96%)	264 (96%)	11 (4%)	31	37
1	M	277/287 (96%)	256 (92%)	21 (8%)	13	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1112/1148 (97%)	1050 (94%)	62 (6%)	21	21

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	LEU
1	A	295	SER
1	A	317	LEU
1	A	422	LYS
1	A	431	LEU
1	A	439	SER
1	A	506	PHE
1	A	534	THR
1	A	536	VAL
1	A	538	ARG
1	A	541	HIS
1	A	544	LYS
1	A	576	LEU
1	A	577	GLU
1	E	254	LEU
1	E	401	LYS
1	E	404	GLN
1	E	413	VAL
1	E	436	ASP
1	E	444	PHE
1	E	467	ASN
1	E	492	ILE
1	E	503	LEU
1	E	514	ARG
1	E	534	THR
1	E	536	VAL
1	E	545	VAL
1	E	549	ARG
1	E	561	ARG
1	E	576	LEU
1	I	254	LEU
1	I	260	LEU
1	I	317	LEU
1	I	354	GLN
1	I	389	ARG
1	I	445	SER
1	I	503	LEU

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Mol	Chain	Res	Type
1	I	519	LEU
1	I	537	VAL
1	I	540	THR
1	I	579	HIS
1	M	250	THR
1	M	259	LYS
1	M	286	LEU
1	M	293	VAL
1	M	302	ILE
1	M	317	LEU
1	M	354	GLN
1	M	385	GLU
1	M	411	LEU
1	M	438	ARG
1	M	449	ASP
1	M	458	THR
1	M	488	ARG
1	M	489	LEU
1	M	493	VAL
1	M	494	VAL
1	M	503	LEU
1	M	541	HIS
1	M	544	LYS
1	M	565	LEU
1	M	568	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	340	ASN
1	A	372	GLN
1	A	373	GLN
1	A	397	GLN
1	A	511	HIS
1	A	541	HIS
1	A	578	HIS
1	A	580	HIS
1	E	290	HIS
1	E	404	GLN
1	E	530	HIS
1	I	253	ASN

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Mol	Chain	Res	Type
1	I	270	GLN
1	I	354	GLN
1	I	372	GLN
1	I	397	GLN
1	I	470	GLN
1	M	255	HIS
1	M	400	GLN
1	M	404	GLN
1	M	470	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 35 ligands modelled in this entry, 23 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	1RY	A	601	6	22,29,29	1.30	3 (13%)	28,45,45	1.54	5 (17%)
7	ACT	I	605	-	1,3,3	2.53	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	1RY	M	601	6	22,29,29	0.97	1 (4%)	28,45,45	1.97	7 (25%)
7	ACT	M	607	-	1,3,3	3.20	1 (100%)	0,3,3	0.00	-
7	ACT	E	608	-	1,3,3	1.69	0	0,3,3	0.00	-
8	CAC	E	607	-	0,4,4	0.00	-	0,6,6	0.00	-
7	ACT	A	608	-	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
5	1RY	I	601	6	22,29,29	0.84	0	28,45,45	1.60	6 (21%)
7	ACT	B	102	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
8	CAC	M	606	-	0,4,4	0.00	-	0,6,6	0.00	-
7	ACT	F	102	-	1,3,3	2.40	1 (100%)	0,3,3	0.00	-
5	1RY	E	601	6	22,29,29	0.99	2 (9%)	28,45,45	1.48	4 (14%)

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	1RY	E	601	6	-	4/19/31/31	0/2/2/2
5	1RY	I	601	6	-	5/19/31/31	0/2/2/2
5	1RY	A	601	6	-	3/19/31/31	0/2/2/2
5	1RY	M	601	6	-	7/19/31/31	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	1RY	CAV-NAN	-3.68	1.30	1.38
7	M	607	ACT	CH3-C	3.20	1.52	1.48
5	A	601	1RY	CAM-SAS	-2.56	1.73	1.81
7	I	605	ACT	CH3-C	2.53	1.52	1.48
5	E	601	1RY	CAT-CAU	-2.44	1.37	1.40
7	F	102	ACT	CH3-C	2.40	1.51	1.48
7	A	608	ACT	CH3-C	2.06	1.51	1.48
5	A	601	1RY	CAX-NAY	-2.03	1.43	1.49
5	E	601	1RY	CAM-SAS	-2.03	1.75	1.81
7	B	102	ACT	CH3-C	2.01	1.51	1.48
5	M	601	1RY	CAM-SAS	-2.01	1.75	1.81

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	1RY	PBB-OAQ-PAZ	-6.83	109.38	132.83
5	I	601	1RY	FAJ-CAU-CAT	4.18	124.37	119.60
5	E	601	1RY	NAA-CAT-NAN	3.42	121.87	117.03
5	A	601	1RY	CAU-CAT-NAA	-3.36	118.71	121.47
5	E	601	1RY	CAU-CAT-NAA	-3.33	118.73	121.47
5	A	601	1RY	NAA-CAT-NAN	3.12	121.45	117.03
5	E	601	1RY	CAV-NAN-CAT	3.12	119.78	116.02
5	M	601	1RY	CAV-NAN-CAT	2.97	119.61	116.02
5	I	601	1RY	CAV-NAN-CAT	2.94	119.57	116.02
5	I	601	1RY	OAF-PAZ-OAC	2.78	118.25	107.64
5	I	601	1RY	PBB-OAQ-PAZ	-2.77	123.32	132.83
5	I	601	1RY	PBA-OAR-PBB	-2.72	123.50	132.83
5	A	601	1RY	PBB-OAQ-PAZ	-2.71	123.53	132.83
5	M	601	1RY	CAU-CAT-NAA	2.64	123.64	121.47
5	M	601	1RY	OAF-PAZ-OAC	2.60	117.58	107.64
5	M	601	1RY	CAW-OAP-CAX	-2.60	107.10	112.59
5	M	601	1RY	OAP-CAX-CAM	-2.58	103.27	109.29
5	A	601	1RY	CAX-CAM-SAS	2.48	109.91	104.03
5	M	601	1RY	CAM-CAX-NAY	-2.39	105.13	112.58
5	A	601	1RY	OAD-PBA-OAO	2.37	118.74	107.75
5	E	601	1RY	OAF-PAZ-OAC	2.03	115.39	107.64
5	I	601	1RY	CAM-SAS-CAW	2.02	93.55	88.24

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	601	1RY	PBB-OAQ-PAZ-OAF
5	M	601	1RY	OAO-CAL-CAW-OAP
5	M	601	1RY	OAP-CAX-NAY-CAK
5	A	601	1RY	PBB-OAQ-PAZ-OAF
5	I	601	1RY	PBB-OAQ-PAZ-OAC
5	I	601	1RY	PBB-OAQ-PAZ-OAF
5	M	601	1RY	OAO-CAL-CAW-SAS
5	M	601	1RY	PAZ-OAQ-PBB-OAE
5	M	601	1RY	PBB-OAQ-PAZ-OAF
5	I	601	1RY	PBA-OAR-PBB-OAE
5	I	601	1RY	OAO-CAL-CAW-OAP
5	M	601	1RY	PAZ-OAQ-PBB-OAI
5	E	601	1RY	PBA-OAR-PBB-OAE
5	E	601	1RY	PBB-OAQ-PAZ-OAG
5	A	601	1RY	PBB-OAQ-PAZ-OAG
5	E	601	1RY	PBB-OAQ-PAZ-OAC

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Mol	Chain	Res	Type	Atoms
5	A	601	1RY	CAL-OAO-PBA-OAR
5	I	601	1RY	CAL-OAO-PBA-OAR
5	M	601	1RY	CAL-OAO-PBA-OAH

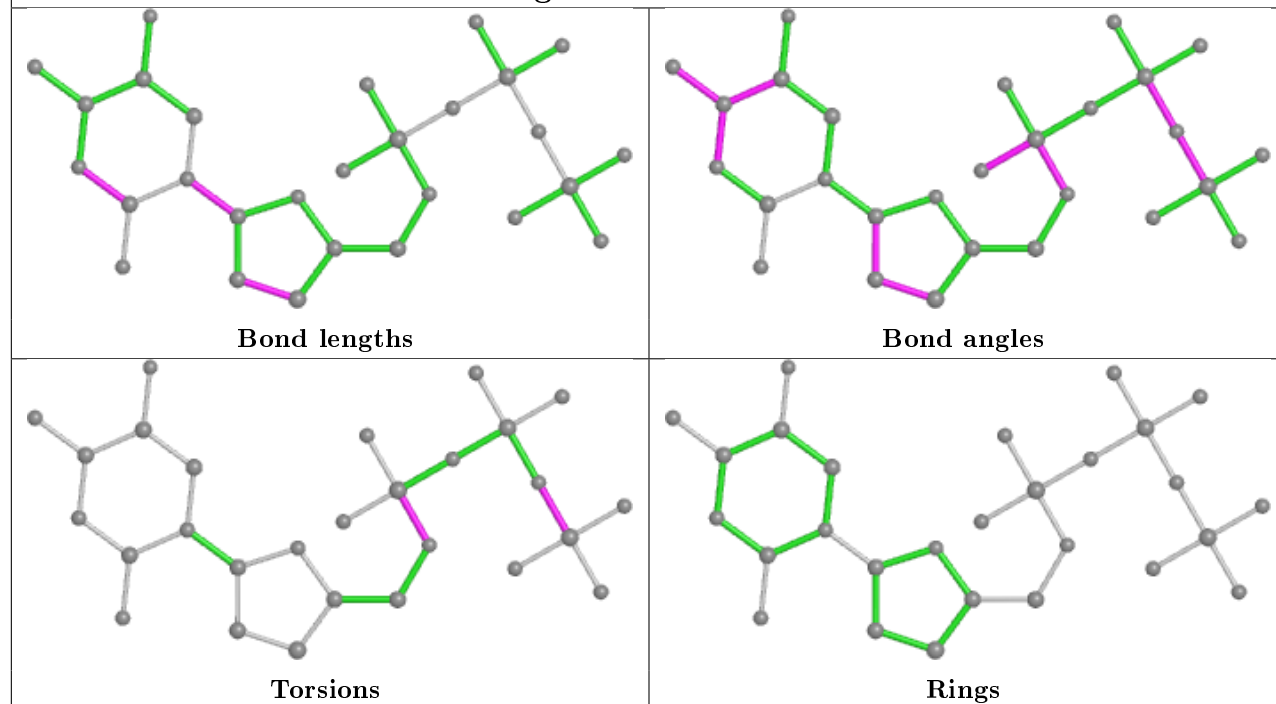
There are no ring outliers.

3 monomers are involved in 5 short contacts:

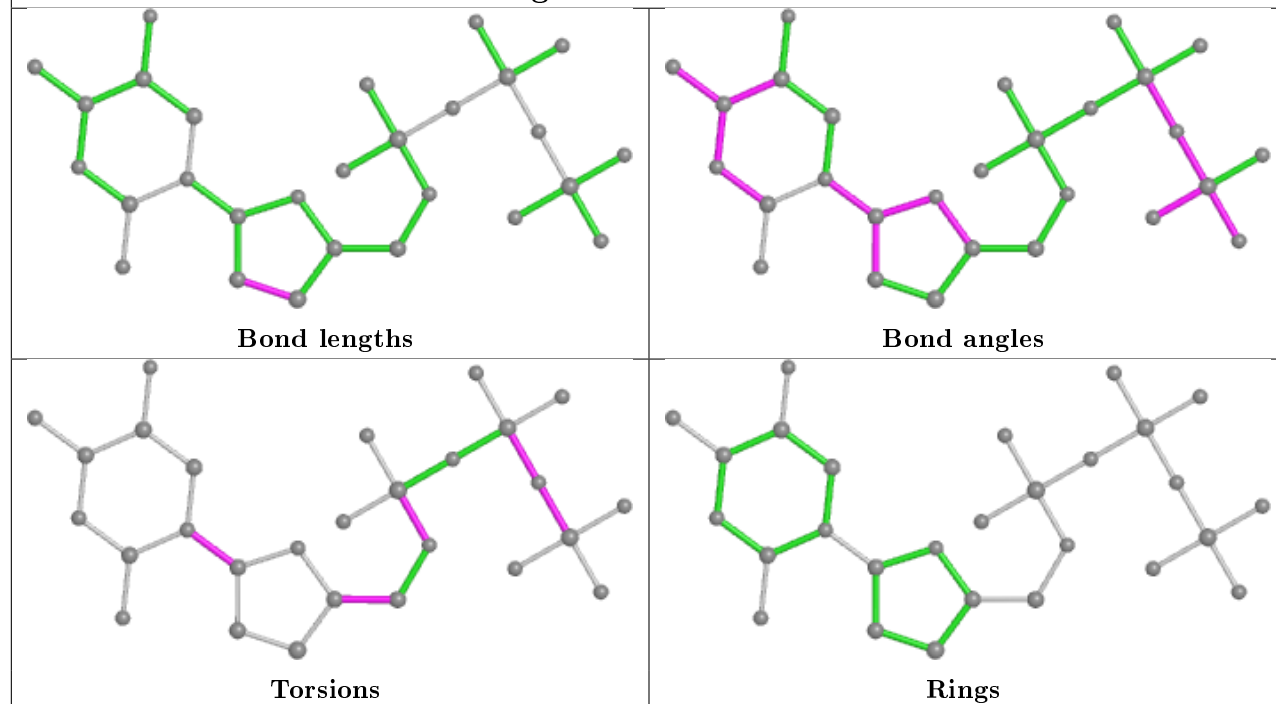
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	601	1RY	1	0
7	E	608	ACT	1	0
8	M	606	CAC	3	0

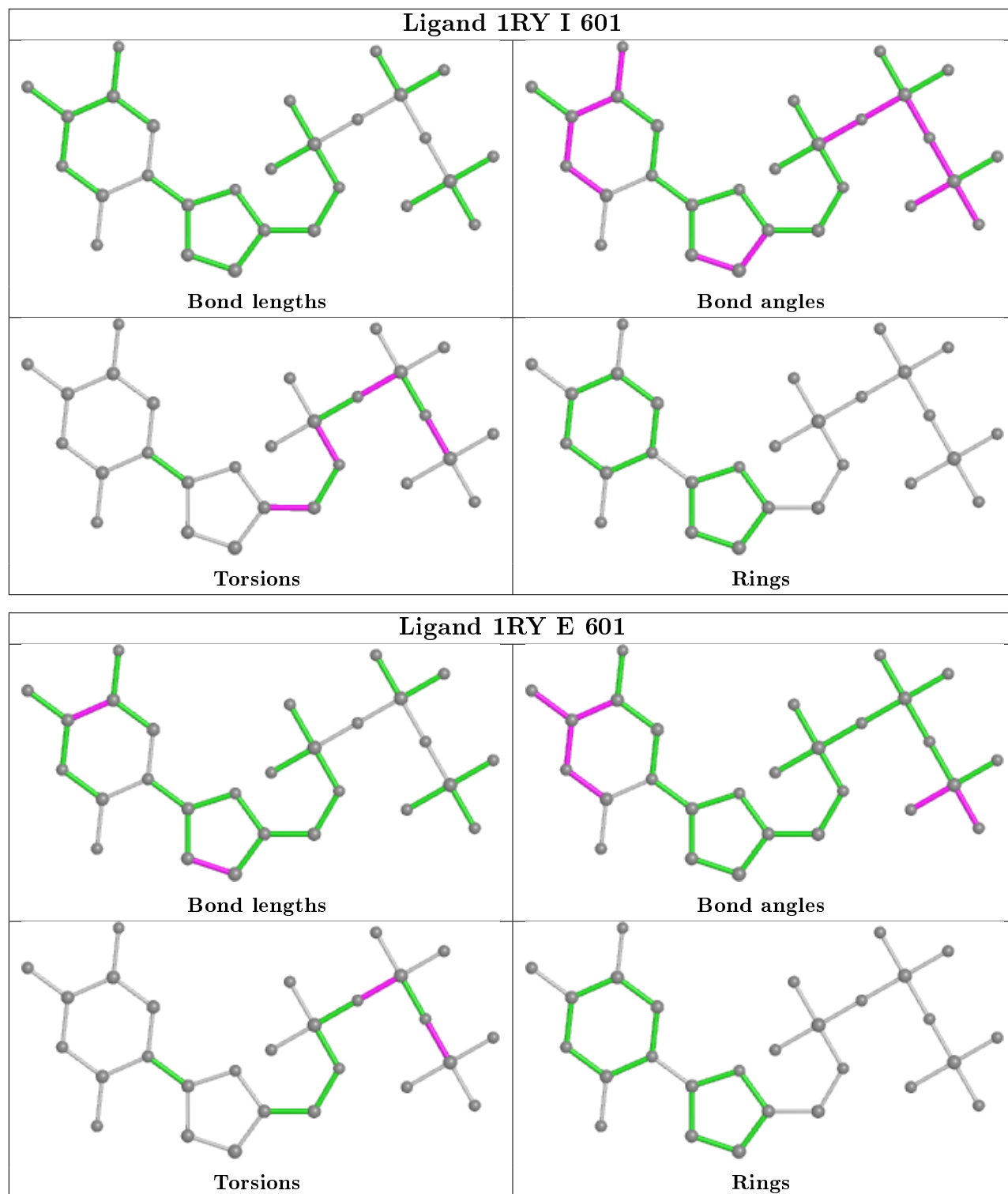
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 1RY A 601



## Ligand 1RY M 601





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	333/340 (97%)	-0.07	17 (5%) 28 30	17, 32, 69, 132	0
1	E	329/340 (96%)	-0.08	11 (3%) 46 48	20, 37, 75, 127	0
1	I	325/340 (95%)	-0.17	12 (3%) 41 44	19, 37, 63, 95	0
1	M	329/340 (96%)	-0.13	13 (3%) 38 40	15, 33, 56, 112	0
2	B	11/11 (100%)	-0.54	0 100 100	21, 25, 42, 46	0
2	F	11/11 (100%)	-0.45	0 100 100	36, 43, 55, 60	0
2	J	11/11 (100%)	-0.49	0 100 100	33, 35, 42, 43	0
2	N	11/11 (100%)	-0.56	0 100 100	22, 29, 40, 44	0
3	C	6/6 (100%)	-0.42	0 100 100	20, 24, 37, 39	0
3	G	6/6 (100%)	-0.18	0 100 100	28, 32, 57, 68	0
3	K	6/6 (100%)	-0.33	0 100 100	23, 25, 64, 69	0
3	O	6/6 (100%)	-0.67	0 100 100	24, 28, 47, 50	0
4	D	4/4 (100%)	-0.87	0 100 100	33, 35, 37, 39	0
4	H	4/4 (100%)	-0.69	0 100 100	28, 32, 33, 37	0
4	L	4/4 (100%)	-0.56	0 100 100	36, 38, 44, 46	0
4	P	4/4 (100%)	-0.88	0 100 100	32, 36, 41, 44	0
All	All	1400/1444 (96%)	-0.14	53 (3%) 40 43	15, 35, 66, 132	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	ARG	8.0
1	A	540	THR	7.5
1	M	249	ALA	6.1
1	M	543	CYS	5.8
1	M	542	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	M	539	ASN	5.7
1	A	541	HIS	5.1
1	I	580	HIS	4.9
1	E	540	THR	4.7
1	A	539	ASN	4.6
1	M	538	ARG	4.4
1	M	541	HIS	4.2
1	A	581	HIS	4.1
1	A	582	HIS	3.9
1	I	321	HIS	3.8
1	M	545	VAL	3.7
1	E	467	ASN	3.6
1	A	542	GLY	3.5
1	I	255	HIS	3.4
1	E	539	ASN	3.3
1	E	541	HIS	3.3
1	A	543	CYS	3.1
1	M	537	VAL	3.0
1	A	323	ARG	2.8
1	I	538	ARG	2.8
1	M	250	THR	2.8
1	I	539	ASN	2.8
1	A	545	VAL	2.7
1	A	580	HIS	2.7
1	A	406	PHE	2.7
1	I	482	PRO	2.6
1	A	328	ILE	2.6
1	I	540	THR	2.6
1	A	537	VAL	2.5
1	I	323	ARG	2.5
1	A	546	GLY	2.5
1	E	576	LEU	2.4
1	M	536	VAL	2.4
1	I	551	LEU	2.4
1	M	575	TRP	2.3
1	E	568	ARG	2.3
1	E	562	LEU	2.2
1	E	543	CYS	2.2
1	I	314	ILE	2.2
1	M	540	THR	2.2
1	E	551	LEU	2.2
1	M	285	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	537	VAL	2.1
1	I	256	ILE	2.1
1	A	255	HIS	2.1
1	A	327	HIS	2.0
1	E	535	ALA	2.0
1	E	518	ALA	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
8	CAC	E	607	5/5	0.53	0.32	132,134,146,155	0
7	ACT	M	607	4/4	0.60	0.22	55,55,57,61	0
6	CA	M	604	1/1	0.60	0.10	49,49,49,49	0
6	CA	J	101	1/1	0.72	0.07	58,58,58,58	0
6	CA	A	607	1/1	0.83	0.16	59,59,59,59	0
6	CA	M	605	1/1	0.84	0.11	61,61,61,61	0
6	CA	K	101	1/1	0.85	0.14	64,64,64,64	0
6	CA	I	604	1/1	0.85	0.11	64,64,64,64	0
7	ACT	E	608	4/4	0.86	0.18	54,55,57,58	0
6	CA	M	602	1/1	0.87	0.15	65,65,65,65	0
6	CA	E	603	1/1	0.89	0.06	50,50,50,50	0
6	CA	E	604	1/1	0.89	0.08	64,64,64,64	0
7	ACT	B	102	4/4	0.89	0.17	48,49,49,57	0
6	CA	E	606	1/1	0.91	0.11	62,62,62,62	0
6	CA	E	605	1/1	0.92	0.18	39,39,39,39	0
8	CAC	M	606	5/5	0.92	0.12	74,77,82,88	0
6	CA	A	602	1/1	0.92	0.17	33,33,33,33	0

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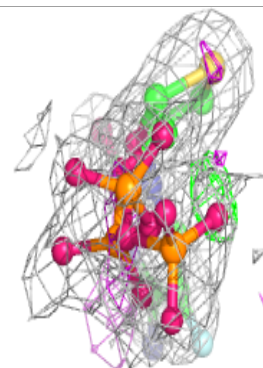
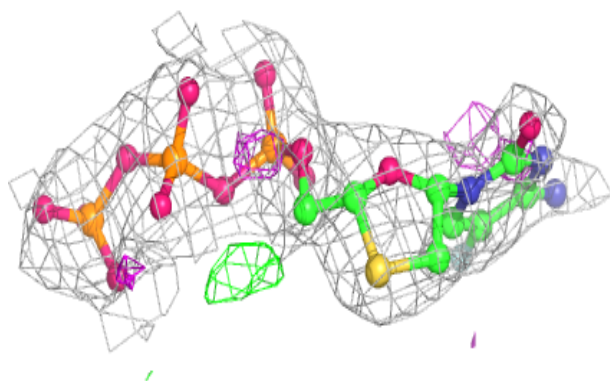
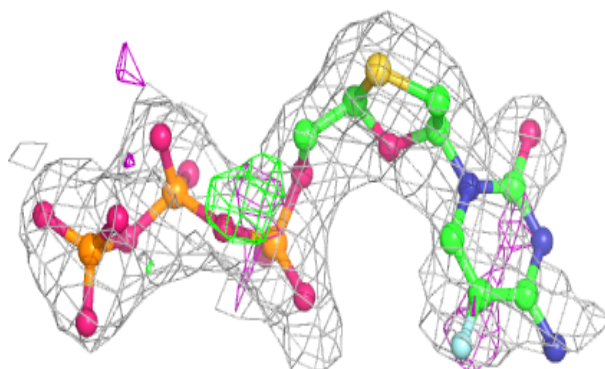
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ACT	I	605	4/4	0.92	0.24	39,43,45,49	0
6	CA	N	101	1/1	0.92	0.07	58,58,58,58	0
7	ACT	F	102	4/4	0.92	0.17	43,48,48,50	0
6	CA	A	606	1/1	0.93	0.06	29,29,29,29	0
6	CA	M	603	1/1	0.93	0.10	42,42,42,42	0
6	CA	F	101	1/1	0.93	0.05	47,47,47,47	0
7	ACT	A	608	4/4	0.93	0.19	41,41,45,51	0
6	CA	A	603	1/1	0.93	0.15	53,53,53,53	0
5	1RY	I	601	28/28	0.94	0.15	41,52,65,66	0
6	CA	I	603	1/1	0.94	0.08	38,38,38,38	0
6	CA	B	101	1/1	0.95	0.16	66,66,66,66	0
5	1RY	M	601	28/28	0.95	0.11	23,32,43,47	0
6	CA	A	604	1/1	0.97	0.03	37,37,37,37	0
5	1RY	E	601	28/28	0.98	0.10	23,32,36,40	0
5	1RY	A	601	28/28	0.98	0.11	18,20,23,24	0
6	CA	A	605	1/1	0.98	0.08	21,21,21,21	0
6	CA	E	602	1/1	0.99	0.10	30,30,30,30	0
6	CA	I	602	1/1	0.99	0.14	35,35,35,35	0

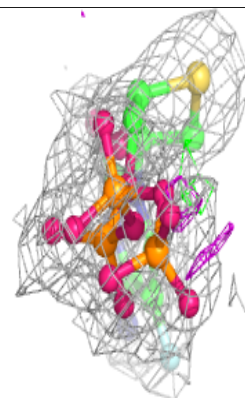
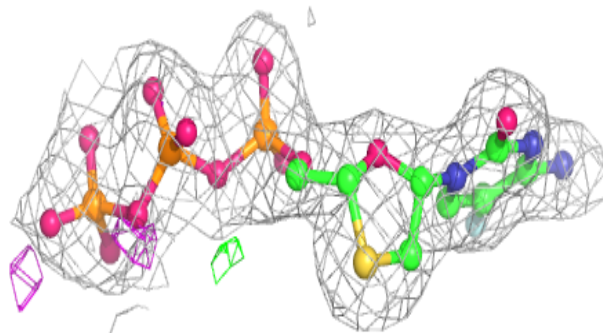
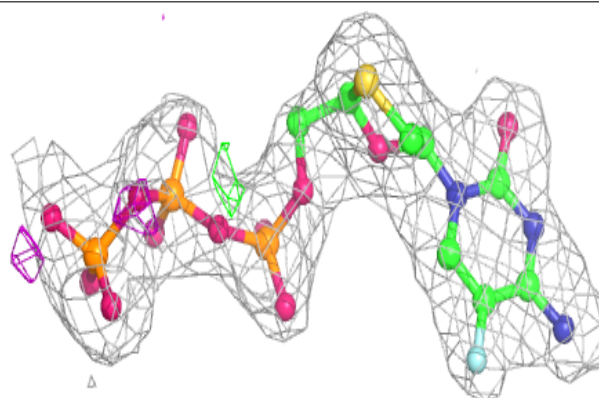
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 1RY 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)

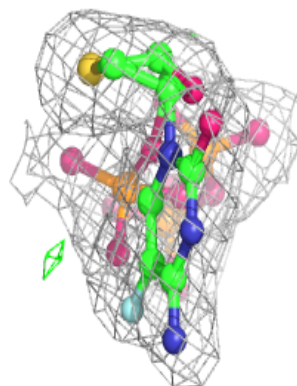
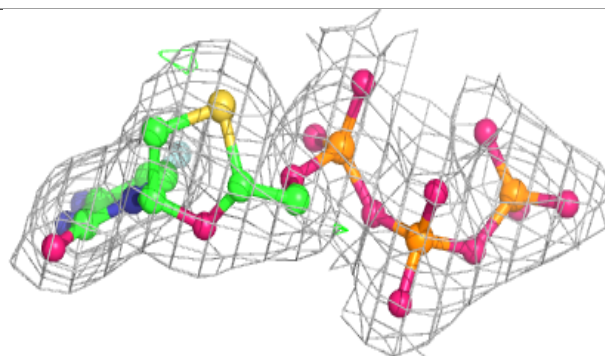
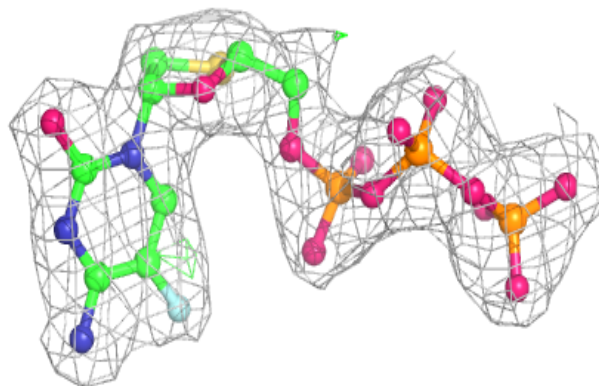
**Electron density around 1RY M 601:**

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

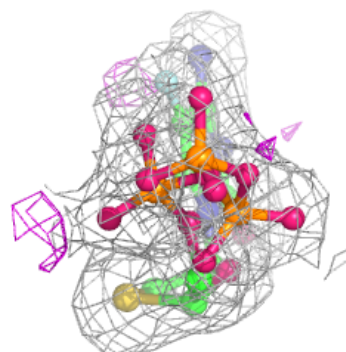
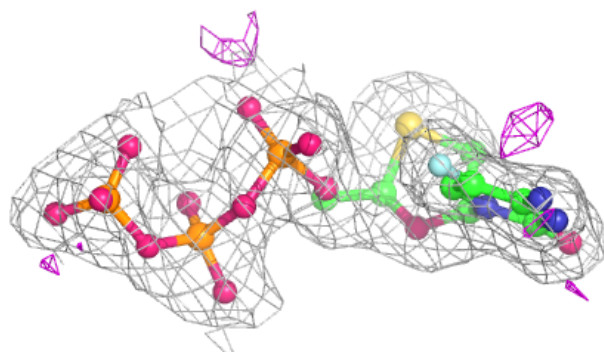
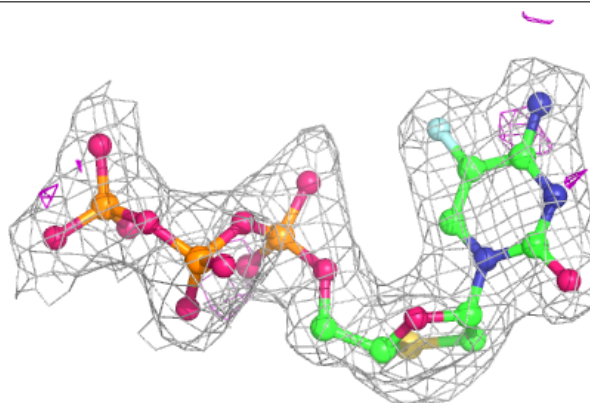


**Electron density around 1RY E 601:**

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

**Electron density around 1RY 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.