



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2021 – 10:11 PM EDT

PDB ID : 3HX0  
Title : ternary complex of L277A, H511A, R514 mutant pol lambda bound to a 2 nucleotide gapped DNA substrate with a scrunched dA  
Authors : Garcia-Diaz, M.; Bebenek, K.; Larrea, A.A.; Havener, J.M.; Perera, L.; Krahn, J.M.; Pedersen, L.C.; Ramsden, D.A.; Kunkel, T.A.  
Deposited on : 2009-06-19  
Resolution : 3.00 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 : 2.23.2  
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) : 2.23.2

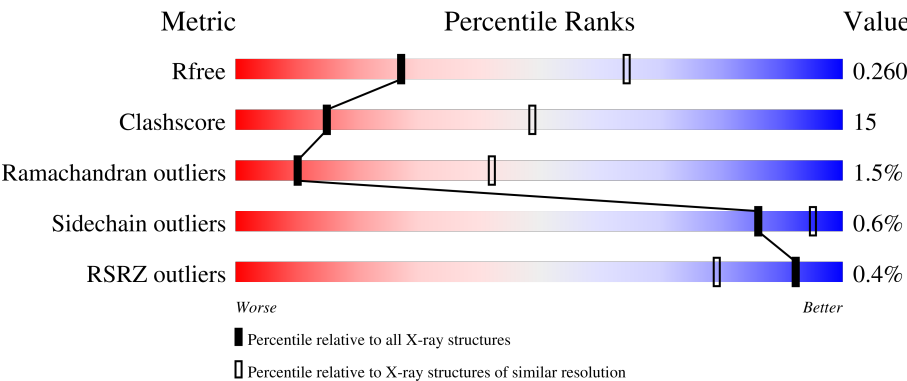
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	335	<div> <div></div> <div>76%</div> <div>22%</div> <div>..</div> </div>
1	F	335	<div> <div></div> <div>68%</div> <div>29%</div> <div>..</div> </div>
1	K	335	<div> <div></div> <div>66%</div> <div>31%</div> <div>..</div> </div>
1	P	335	<div> <div></div> <div>58%</div> <div>39%</div> <div>..</div> </div>
2	B	12	<div> <div></div> <div>42%</div> <div>58%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	12	 42%58%
2	L	12	 58%42%
2	Q	12	 42%58%
3	C	6	 100%
3	H	6	 67%33%
3	M	6	 83%17%
3	R	6	 83%17%
4	D	4	 75%25%
4	I	4	 75%25%
4	N	4	 75%25%
4	S	4	 25%50%25%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11946 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	330	Total	C	N	O	S	0	0	0
			2511	1577	455	468	11			
1	F	329	Total	C	N	O	S	0	0	0
			2520	1583	456	470	11			
1	K	327	Total	C	N	O	S	0	0	0
			2505	1573	454	467	11			
1	P	327	Total	C	N	O	S	0	0	0
			2470	1550	444	465	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	initiating methionine	UNP Q9UGP5
A	277	ALA	LEU	engineered mutation	UNP Q9UGP5
A	511	ALA	HIS	engineered mutation	UNP Q9UGP5
A	514	ALA	ARG	engineered mutation	UNP Q9UGP5
A	543	ALA	CYS	engineered mutation	UNP Q9UGP5
F	241	MET	-	initiating methionine	UNP Q9UGP5
F	277	ALA	LEU	engineered mutation	UNP Q9UGP5
F	511	ALA	HIS	engineered mutation	UNP Q9UGP5
F	514	ALA	ARG	engineered mutation	UNP Q9UGP5
F	543	ALA	CYS	engineered mutation	UNP Q9UGP5
K	241	MET	-	initiating methionine	UNP Q9UGP5
K	277	ALA	LEU	engineered mutation	UNP Q9UGP5
K	511	ALA	HIS	engineered mutation	UNP Q9UGP5
K	514	ALA	ARG	engineered mutation	UNP Q9UGP5
K	543	ALA	CYS	engineered mutation	UNP Q9UGP5
P	241	MET	-	initiating methionine	UNP Q9UGP5
P	277	ALA	LEU	engineered mutation	UNP Q9UGP5
P	511	ALA	HIS	engineered mutation	UNP Q9UGP5
P	514	ALA	ARG	engineered mutation	UNP Q9UGP5
P	543	ALA	CYS	engineered mutation	UNP Q9UGP5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			244	117	48	68	11			
2	G	12	Total	C	N	O	P	0	0	0
			244	117	48	68	11			
2	L	12	Total	C	N	O	P	0	0	0
			244	117	48	68	11			
2	Q	12	Total	C	N	O	P	0	0	0
			244	117	48	68	11			

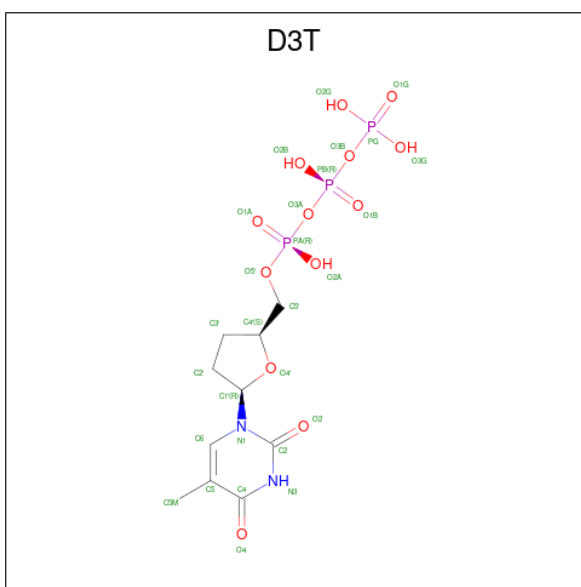
- Molecule 3 is a DNA chain called 5'-D(\*CP\*AP\*GP\*TP\*AP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	P	0	0	0
			119	59	22	33	5			
3	H	6	Total	C	N	O	P	0	0	0
			119	59	22	33	5			
3	M	6	Total	C	N	O	P	0	0	0
			119	59	22	33	5			
3	R	6	Total	C	N	O	P	0	0	0
			119	59	22	33	5			

- Molecule 4 is a DNA chain called 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	I	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
4	N	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
4	S	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

- Molecule 5 is 2',3'-DIDEOXY-THYMIDINE-5'-TRIPHOSPHATE (three-letter code: D3T) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>2</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 28	C 10	N 2	O 13	P 3	0	0
5	F	1	Total 28	C 10	N 2	O 13	P 3	0	0
5	K	1	Total 28	C 10	N 2	O 13	P 3	0	0
5	P	1	Total 28	C 10	N 2	O 13	P 3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0
6	K	1	Total Mg 1 1	0	0
6	P	1	Total Mg 1 1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	2	Total 2	Na 2	0	0
7	P	2	Total 2	Na 2	0	0

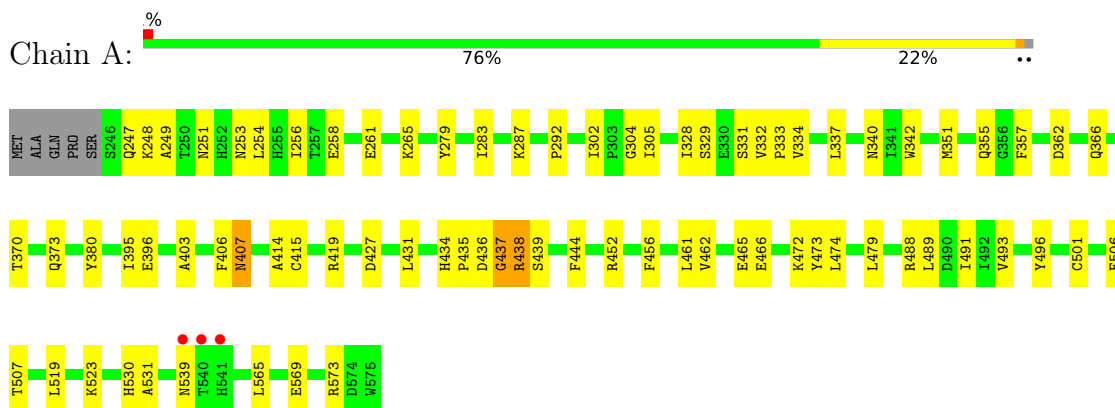
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	10	Total 10	O 10	0	0
8	B	1	Total 1	O 1	0	0
8	F	6	Total 6	O 6	0	0
8	G	2	Total 2	O 2	0	0
8	K	11	Total 11	O 11	0	0
8	L	1	Total 1	O 1	0	0
8	P	4	Total 4	O 4	0	0

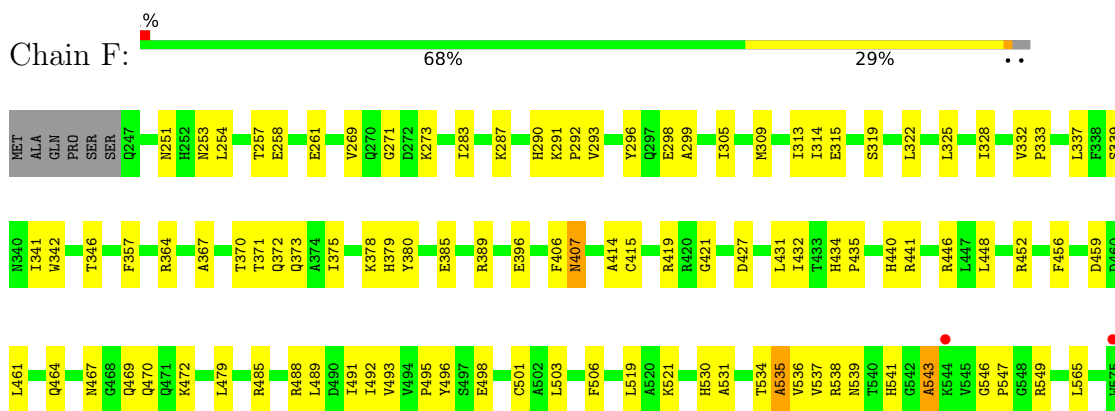
### 3 Residue-property plots

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.

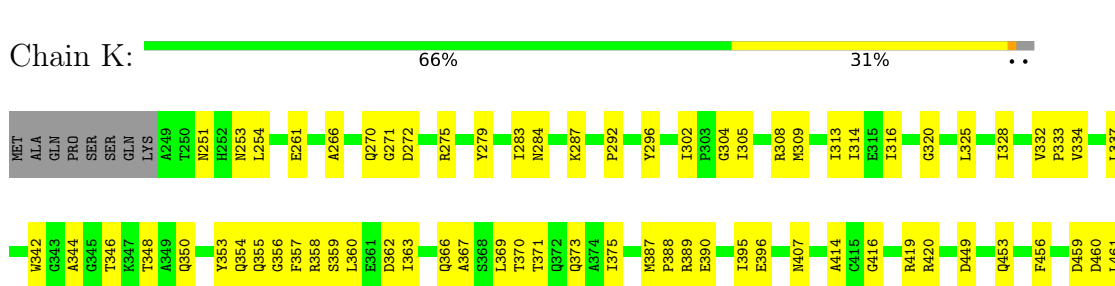
- Molecule 1: DNA polymerase lambda



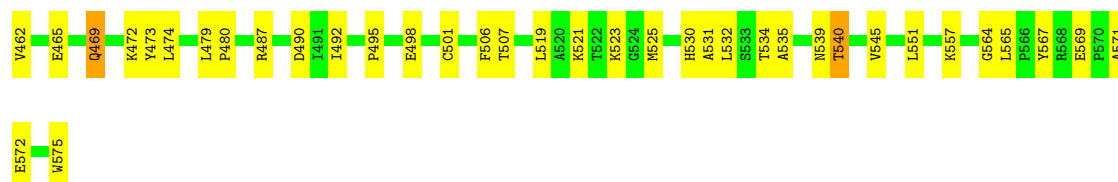
- Molecule 1: DNA polymerase lambda



- Molecule 1: DNA polymerase lambda

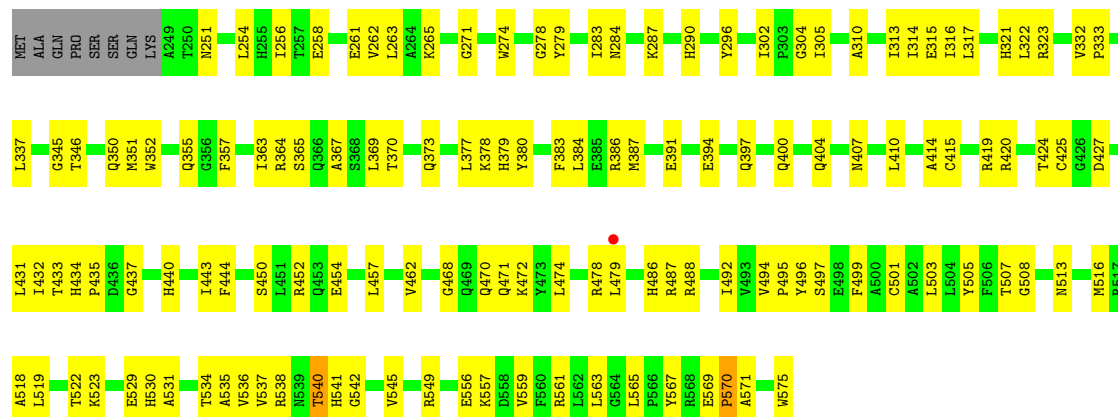






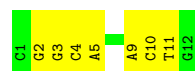
- Molecule 1: DNA polymerase lambda

Chain P: 58% 39% ..



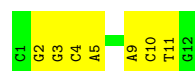
- Molecule 2: 5'-D(\*CP\*GP\*GP\*CP\*AP\*AP\*AP\*TP\*AP\*CP\*TP\*G)-3'

Chain B: 42% 58%



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

Chain G: 42% 58%



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

Chain L: 58% 42%



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

Chain Q: 42% 58%



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

Chain C: 100%

There are no outlier residues recorded for this chain.

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

Chain H: 67% 33%



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

Chain M: 83% 17%



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

Chain R: 83% 17%



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

Chain D: 75% 25%



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

Chain I: 75% 25%



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

Chain N: 75% 25%



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

Chain S:  25% 50% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.18Å 131.91Å 280.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.11 – 3.00 48.04 – 3.03	Depositor EDS
% Data completeness (in resolution range)	94.5 (39.11-3.00) 94.5 (48.04-3.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.223 , 0.268 0.216 , 0.260	Depositor DCC
$R_{free}$ test set	2208 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: MG, NA, D3T

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	0.25	0/2563	0.47	0/3469
1	F	0.26	0/2571	0.46	0/3479
1	K	0.25	0/2556	0.47	0/3460
1	P	0.26	0/2518	0.47	0/3414
2	B	0.20	0/274	0.66	0/421
2	G	0.23	0/274	0.72	0/421
2	L	0.22	0/274	0.65	0/421
2	Q	0.24	0/274	0.72	0/421
3	C	0.22	0/133	0.66	0/203
3	H	0.24	0/133	0.69	0/203
3	M	0.24	0/133	0.70	0/203
3	R	0.24	0/133	0.71	0/203
4	D	0.92	1/92 (1.1%)	0.71	0/138
4	I	0.93	1/92 (1.1%)	0.73	0/138
4	N	0.94	1/92 (1.1%)	0.77	0/138
4	S	0.93	1/92 (1.1%)	0.73	0/138
All	All	0.29	4/12204 (0.0%)	0.52	0/16870

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1	DG	OP3-P	-7.38	1.52	1.61
4	D	1	DG	OP3-P	-7.28	1.52	1.61
4	I	1	DG	OP3-P	-7.27	1.52	1.61
4	N	1	DG	OP3-P	-7.23	1.52	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	2511	0	2433	50	0
1	F	2520	0	2457	74	0
1	K	2505	0	2442	80	0
1	P	2470	0	2389	104	0
2	B	244	0	136	6	0
2	G	244	0	136	8	0
2	L	244	0	136	3	0
2	Q	244	0	136	6	0
3	C	119	0	68	0	0
3	H	119	0	68	4	0
3	M	119	0	68	1	0
3	R	119	0	68	1	0
4	D	83	0	45	4	0
4	I	83	0	45	3	0
4	N	83	0	45	5	0
4	S	83	0	45	3	0
5	A	28	0	13	0	0
5	F	28	0	13	0	0
5	K	28	0	13	1	0
5	P	28	0	13	0	0
6	A	1	0	0	0	0
6	F	1	0	0	0	0
6	K	1	0	0	0	0
6	P	1	0	0	0	0
7	F	1	0	0	0	0
7	K	2	0	0	0	0
7	P	2	0	0	0	0
8	A	10	0	0	0	0
8	B	1	0	0	0	0
8	F	6	0	0	0	0
8	G	2	0	0	0	0
8	K	11	0	0	0	0
8	L	1	0	0	0	0
8	P	4	0	0	0	0
All	All	11946	0	10769	342	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 15.

All (342) 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:P:431:LEU:HG	1:P:492:ILE:HD11	1.46	0.94
1:K:348:THR:HG21	1:K:373:GLN:HE22	1.34	0.93
1:P:346:THR:HG22	1:P:350:GLN:HE21	1.40	0.86
1:P:519:LEU:HD13	1:P:565:LEU:HD21	1.57	0.84
1:F:254:LEU:O	1:F:258:GLU:HB2	1.81	0.81
2:B:10:DC:H2''	2:B:11:DT:H5'	1.63	0.80
1:K:346:THR:HG22	1:K:350:GLN:HE21	1.46	0.79
1:F:396:GLU:HG3	1:F:414:ALA:HB2	1.64	0.77
1:P:254:LEU:O	1:P:258:GLU:HB2	1.86	0.76
1:P:470:GLN:HG2	1:P:494:VAL:HG12	1.68	0.76
1:K:501:CYS:SG	1:K:531:ALA:HA	2.25	0.75
1:K:519:LEU:HD13	1:K:565:LEU:HD21	1.69	0.74
4:I:3:DC:H2''	4:I:4:DG:H5'	1.69	0.74
1:A:251:ASN:ND2	1:A:287:LYS:HG2	2.03	0.73
1:A:254:LEU:O	1:A:258:GLU:HG3	1.91	0.71
1:K:296:TYR:HB2	1:K:314:ILE:HG13	1.73	0.69
1:A:519:LEU:HD23	1:A:565:LEU:HD11	1.74	0.69
1:F:519:LEU:HD23	1:F:565:LEU:HD11	1.77	0.67
1:A:434:HIS:O	1:A:496:TYR:HB2	1.93	0.67
1:F:332:VAL:HB	1:F:333:PRO:HD3	1.76	0.67
1:K:332:VAL:HB	1:K:333:PRO:HD3	1.77	0.67
1:P:345:GLY:N	3:R:5:DA:H5''	2.10	0.66
1:P:501:CYS:SG	1:P:531:ALA:HA	2.35	0.66
3:H:5:DA:H2''	3:H:6:DT:O5'	1.96	0.64
1:F:537:VAL:HB	1:F:546:GLY:H	1.62	0.64
1:A:357:PHE:HE1	1:A:366:GLN:HB2	1.62	0.64
1:F:501:CYS:SG	1:F:531:ALA:HA	2.38	0.64
1:K:348:THR:HG21	1:K:373:GLN:NE2	2.09	0.63
1:A:370:THR:OG1	1:A:373:GLN:HG3	1.99	0.63
1:P:559:VAL:O	1:P:563:LEU:HB2	1.98	0.63
2:B:5:DA:N3	2:B:5:DA:H2'	2.13	0.63
1:P:363:ILE:O	1:P:367:ALA:HB3	1.99	0.63
1:K:296:TYR:N	1:K:314:ILE:HD11	2.15	0.62
1:P:346:THR:HG22	1:P:350:GLN:NE2	2.12	0.62
1:F:385:GLU:HG3	1:F:485:ARG:NH1	2.14	0.62
1:K:449:ASP:O	1:K:453:GLN:HG2	2.00	0.62
1:A:415:CYS:HA	1:A:419:ARG:HB2	1.81	0.61
1:P:332:VAL:HB	1:P:333:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:370:THR:OG1	1:P:373:GLN:HG3	2.00	0.60
1:K:271:GLY:HA2	1:K:346:THR:HG21	1.83	0.60
1:K:363:ILE:HA	1:K:367:ALA:CB	2.30	0.60
1:P:380:TYR:HE1	1:P:384:LEU:HD11	1.66	0.60
1:K:557:LYS:HG2	1:K:567:TYR:CD2	2.36	0.60
1:F:251:ASN:HD21	1:F:254:LEU:HA	1.67	0.60
1:K:534:THR:HG22	1:K:535:ALA:N	2.18	0.59
1:A:329:SER:C	1:A:331:SER:H	2.06	0.59
1:F:296:TYR:N	1:F:314:ILE:HD11	2.17	0.59
1:K:370:THR:OG1	1:K:373:GLN:HG3	2.02	0.59
1:A:247:GLN:O	1:A:249:ALA:N	2.36	0.59
1:A:519:LEU:CD2	1:A:565:LEU:HD11	2.32	0.59
1:K:359:SER:HB3	1:K:362:ASP:OD1	2.03	0.59
1:A:302:ILE:HB	1:A:305:ILE:HD12	1.85	0.58
1:A:406:PHE:O	1:A:407:ASN:HB2	2.02	0.58
2:Q:2:DG:H2''	2:Q:3:DG:OP2	2.04	0.58
1:P:450:SER:O	1:P:454:GLU:HG2	2.03	0.58
4:N:1:DG:H2''	4:N:2:DC:H5'	1.85	0.58
1:K:316:ILE:O	1:K:320:GLY:HA2	2.02	0.58
1:P:397:GLN:HA	1:P:400:GLN:HB3	1.86	0.58
1:A:436:ASP:OD1	1:A:439:SER:HB2	2.03	0.58
2:B:2:DG:H2''	2:B:3:DG:OP2	2.04	0.57
1:P:256:ILE:HD11	1:P:317:LEU:HD21	1.86	0.57
1:K:251:ASN:OD1	1:K:287:LYS:HA	2.05	0.57
1:P:440:HIS:O	1:P:443:ILE:HG13	2.04	0.57
1:K:283:ILE:HG22	1:K:287:LYS:NZ	2.20	0.57
1:F:378:LYS:HE3	1:F:379:HIS:CE1	2.39	0.57
1:K:525:MET:HE1	1:K:532:LEU:HD21	1.86	0.56
1:F:337:LEU:HD12	1:F:380:TYR:OH	2.05	0.56
1:K:416:GLY:H	1:K:507:THR:HA	1.68	0.56
1:P:400:GLN:HG2	1:P:404:GLN:NE2	2.19	0.56
1:P:387:MET:HE2	1:P:487:ARG:HD2	1.87	0.56
1:K:396:GLU:HG3	1:K:414:ALA:HB2	1.87	0.56
1:P:386:ARG:HB3	1:P:424:THR:HB	1.87	0.56
1:K:363:ILE:HA	1:K:367:ALA:HB3	1.88	0.55
1:P:505:TYR:CD2	1:P:529:GLU:HB3	2.42	0.55
1:A:357:PHE:CE1	1:A:366:GLN:HB2	2.41	0.55
1:K:357:PHE:CE1	1:K:366:GLN:HG3	2.41	0.55
1:K:469:GLN:HB3	1:K:495:PRO:HG2	1.87	0.55
1:P:443:ILE:HD12	1:P:444:PHE:N	2.21	0.55
1:A:501:CYS:SG	1:A:531:ALA:HA	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:473:TYR:C	1:K:474:LEU:HD12	2.28	0.55
1:F:431:LEU:HG	1:F:492:ILE:HD11	1.89	0.55
1:P:316:ILE:HG12	1:P:321:HIS:O	2.06	0.55
1:A:251:ASN:HD21	1:A:287:LYS:HG2	1.72	0.55
1:F:342:TRP:CE2	1:F:461:LEU:HD13	2.42	0.55
1:F:257:THR:HB	1:F:283:ILE:HG23	1.89	0.54
1:F:357:PHE:CE1	1:F:367:ALA:HB2	2.42	0.54
1:P:519:LEU:CD2	1:P:565:LEU:HD11	2.38	0.54
1:A:357:PHE:HD1	1:A:362:ASP:HB3	1.72	0.54
1:K:275:ARG:NH1	4:N:1:DG:H8	2.04	0.54
1:P:492:ILE:O	1:P:492:ILE:HD12	2.07	0.54
2:Q:5:DA:H1'	2:Q:6:DA:H5'	1.89	0.54
1:A:396:GLU:HG3	1:A:414:ALA:HB2	1.89	0.54
1:F:406:PHE:O	1:F:407:ASN:HB2	2.06	0.54
1:F:536:VAL:HB	1:F:538:ARG:NH1	2.23	0.54
1:P:284:ASN:HB3	1:P:575:TRP:CD1	2.42	0.54
1:K:387:MET:HE1	1:K:487:ARG:HB3	1.89	0.54
1:F:315:GLU:O	1:F:319:SER:HB2	2.08	0.54
4:N:1:DG:C2'	4:N:2:DC:H5'	2.37	0.54
1:F:492:ILE:HD12	1:F:492:ILE:O	2.08	0.54
1:F:290:HIS:CE1	1:F:291:LYS:HG2	2.44	0.53
1:F:441:ARG:HG3	1:F:441:ARG:HH11	1.73	0.53
1:P:394:GLU:HB2	1:P:479:LEU:HD11	1.90	0.53
1:F:419:ARG:NH1	1:F:503:LEU:HG	2.23	0.53
3:H:5:DA:C8	3:H:6:DT:H72	2.42	0.53
1:P:314:ILE:HD13	1:P:317:LEU:HD12	1.91	0.53
1:F:519:LEU:HD21	1:F:565:LEU:HD21	1.91	0.53
3:H:5:DA:H2'	3:H:6:DT:C7	2.39	0.53
1:F:251:ASN:ND2	1:F:254:LEU:HA	2.23	0.53
2:G:4:DC:H2''	2:G:5:DA:C2	2.43	0.53
1:K:302:ILE:HB	1:K:305:ILE:HD12	1.90	0.53
1:P:379:HIS:HB2	1:P:383:PHE:CE2	2.43	0.53
1:F:448:LEU:O	1:F:452:ARG:HD2	2.08	0.53
2:G:5:DA:N3	2:G:5:DA:H2'	2.24	0.53
1:P:363:ILE:HA	1:P:367:ALA:HB2	1.91	0.53
1:F:537:VAL:HB	1:F:546:GLY:N	2.23	0.52
1:P:302:ILE:HB	1:P:305:ILE:HD12	1.90	0.52
1:P:313:ILE:O	1:P:317:LEU:HG	2.09	0.52
1:A:337:LEU:HD12	1:A:380:TYR:OH	2.09	0.52
1:F:251:ASN:OD1	1:F:287:LYS:HA	2.08	0.52
1:P:387:MET:HB3	1:P:487:ARG:NE	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:415:CYS:HB3	1:P:507:THR:HA	1.91	0.52
2:B:3:DG:H1'	2:B:4:DC:H5'	1.92	0.52
1:K:251:ASN:ND2	1:K:254:LEU:HA	2.24	0.52
1:P:352:TRP:CZ2	1:P:369:LEU:HD23	2.44	0.52
1:P:364:ARG:HB2	1:P:377:LEU:HD21	1.91	0.52
1:A:283:ILE:HG22	1:A:287:LYS:HE3	1.91	0.52
1:K:465:GLU:HG3	2:L:9:DA:H5'	1.92	0.52
4:I:3:DC:H2'	4:I:4:DG:C8	2.44	0.52
1:P:351:MET:O	1:P:355:GLN:HB2	2.10	0.52
1:P:443:ILE:HD12	1:P:443:ILE:C	2.31	0.52
1:K:271:GLY:CA	1:K:346:THR:HG21	2.39	0.51
1:P:310:ALA:HA	1:P:313:ILE:HD12	1.93	0.51
1:P:386:ARG:CB	1:P:424:THR:HB	2.40	0.51
1:A:427:ASP:HB2	1:A:488:ARG:O	2.10	0.51
1:K:309:MET:O	1:K:313:ILE:HG13	2.10	0.51
1:K:305:ILE:HG23	1:K:309:MET:HB3	1.92	0.51
1:P:258:GLU:O	1:P:262:VAL:HG23	2.11	0.51
1:P:557:LYS:HG2	1:P:567:TYR:CD2	2.45	0.51
2:L:1:DC:H2''	2:L:2:DG:H5'	1.93	0.51
1:F:406:PHE:CE2	1:F:446:ARG:HD3	2.46	0.51
1:F:534:THR:CG2	1:F:549:ARG:HB3	2.40	0.51
1:K:302:ILE:N	1:K:302:ILE:HD12	2.26	0.51
1:P:434:HIS:O	1:P:496:TYR:HB2	2.11	0.51
1:P:508:GLY:HA2	1:P:513:ASN:HD21	1.76	0.51
1:F:322:LEU:HD23	1:F:325:LEU:HG	1.92	0.50
1:P:380:TYR:CE1	1:P:384:LEU:HD11	2.45	0.50
1:A:332:VAL:HB	1:A:333:PRO:HD3	1.93	0.50
1:K:564:GLY:C	1:K:565:LEU:HD12	2.32	0.50
1:P:427:ASP:HB3	1:P:488:ARG:HH11	1.76	0.50
1:P:337:LEU:HD12	1:P:380:TYR:OH	2.11	0.50
1:A:261:GLU:HG3	1:A:265:LYS:NZ	2.25	0.50
1:F:291:LYS:HB2	1:F:292:PRO:HD2	1.93	0.50
1:F:435:PRO:HA	1:F:496:TYR:CD1	2.47	0.50
1:A:569:GLU:O	1:A:573:ARG:HG3	2.12	0.50
1:F:357:PHE:HE1	1:F:367:ALA:HB2	1.75	0.49
1:F:427:ASP:HB2	1:F:488:ARG:O	2.12	0.49
1:K:375:ILE:HD13	1:K:459:ASP:HB3	1.94	0.49
1:P:538:ARG:HB2	1:P:542:GLY:HA2	1.94	0.49
1:P:357:PHE:N	1:P:357:PHE:CD2	2.80	0.49
1:F:389:ARG:HG3	1:F:389:ARG:HH11	1.78	0.49
1:F:456:PHE:HE1	1:F:479:LEU:HD23	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:390:GLU:CD	1:K:390:GLU:H	2.14	0.49
1:K:272:ASP:OD1	1:K:275:ARG:HB2	2.12	0.49
1:K:279:TYR:O	1:K:283:ILE:HG13	2.13	0.49
1:P:516:MET:CE	1:P:563:LEU:HD13	2.43	0.49
1:F:534:THR:O	1:F:535:ALA:C	2.52	0.48
1:K:354:GLN:O	1:K:354:GLN:HG2	2.13	0.48
1:P:536:VAL:HG23	1:P:536:VAL:O	2.14	0.48
1:A:403:ALA:HA	1:A:406:PHE:HE1	1.78	0.48
1:P:314:ILE:C	1:P:316:ILE:H	2.16	0.48
1:F:464:GLN:H	1:F:470:GLN:HE21	1.59	0.48
1:P:433:THR:HG21	1:P:499:PHE:CD1	2.48	0.48
1:P:519:LEU:HD22	1:P:563:LEU:HD22	1.95	0.48
1:P:519:LEU:CD1	1:P:565:LEU:HD21	2.36	0.48
1:K:474:LEU:HG	1:K:490:ASP:OD1	2.13	0.48
1:P:263:LEU:HD23	1:P:279:TYR:HE2	1.79	0.48
1:P:516:MET:HE2	1:P:563:LEU:HD13	1.95	0.48
1:F:464:GLN:O	1:F:470:GLN:HB2	2.14	0.48
4:D:2:DC:H1'	4:D:3:DC:H5'	1.95	0.48
1:K:469:GLN:HB3	1:K:495:PRO:CG	2.44	0.48
1:K:308:ARG:HG2	1:K:308:ARG:HH11	1.79	0.48
1:A:530:HIS:O	1:A:531:ALA:HB2	2.14	0.47
1:A:489:LEU:HD21	1:A:491:ILE:HD11	1.95	0.47
2:G:9:DA:H2''	2:G:10:DC:C5'	2.44	0.47
3:H:5:DA:H2'	3:H:6:DT:H72	1.96	0.47
1:P:518:ALA:O	1:P:522:THR:HG23	2.14	0.47
1:F:472:LYS:HA	1:F:492:ILE:HG22	1.95	0.47
1:P:452:ARG:HB2	1:P:457:LEU:HD12	1.96	0.47
1:P:519:LEU:HD22	1:P:565:LEU:HD11	1.96	0.47
1:P:569:GLU:C	1:P:571:ALA:H	2.18	0.47
1:A:342:TRP:CZ3	1:A:461:LEU:HB3	2.49	0.47
1:F:415:CYS:HA	1:F:419:ARG:HB2	1.95	0.47
2:G:2:DG:H2''	2:G:3:DG:OP2	2.15	0.47
1:A:253:ASN:HB3	1:A:256:ILE:HD12	1.96	0.47
2:L:5:DA:H1'	2:L:6:DA:H5'	1.97	0.47
2:Q:11:DT:H2''	2:Q:12:DG:C8	2.49	0.47
1:F:441:ARG:HG3	1:F:441:ARG:NH1	2.30	0.47
1:F:498:GLU:HG2	1:F:530:HIS:O	2.15	0.47
1:P:274:TRP:HA	1:P:274:TRP:CE3	2.49	0.47
1:P:534:THR:HG22	1:P:549:ARG:N	2.30	0.47
1:A:472:LYS:HE3	2:B:9:DA:H4'	1.97	0.47
1:F:364:ARG:HG2	1:F:364:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:472:LYS:CB	1:F:492:ILE:HG22	2.45	0.46
1:P:387:MET:HG2	1:P:425:CYS:O	2.15	0.46
1:A:351:MET:O	1:A:355:GLN:HG3	2.16	0.46
1:K:253:ASN:OD1	1:K:292:PRO:HA	2.15	0.46
1:P:420:ARG:HA	1:P:570:PRO:O	2.15	0.46
1:F:299:ALA:HB1	1:F:313:ILE:HD12	1.98	0.46
1:F:305:ILE:HG23	1:F:309:MET:HB3	1.96	0.46
1:F:534:THR:HG22	1:F:549:ARG:HB3	1.98	0.46
1:P:519:LEU:HD23	1:P:519:LEU:O	2.16	0.46
4:D:1:DG:H2''	4:D:2:DC:H5'	1.98	0.46
1:K:395:ILE:HG23	1:K:456:PHE:HZ	1.80	0.46
1:P:279:TYR:O	1:P:283:ILE:HG13	2.16	0.46
1:P:304:GLY:O	4:S:2:DC:H4'	2.15	0.46
1:A:395:ILE:HG23	1:A:456:PHE:HZ	1.80	0.45
1:A:456:PHE:HE1	1:A:479:LEU:HD23	1.81	0.45
4:D:3:DC:H2''	4:D:4:DG:C8	2.51	0.45
1:F:534:THR:HG22	1:F:549:ARG:O	2.15	0.45
1:K:266:ALA:O	1:K:270:GLN:HG3	2.16	0.45
1:P:462:VAL:HG21	1:P:474:LEU:HD12	1.97	0.45
1:P:478:ARG:HD3	1:P:486:HIS:CD2	2.50	0.45
2:B:10:DC:H2''	2:B:11:DT:C5'	2.41	0.45
1:F:269:VAL:O	1:F:346:THR:HG23	2.16	0.45
1:K:534:THR:HG22	1:K:535:ALA:H	1.81	0.45
1:P:472:LYS:HA	1:P:492:ILE:HG22	1.98	0.45
1:F:375:ILE:HD13	1:F:459:ASP:HB3	1.98	0.45
1:F:541:HIS:CB	1:K:540:THR:HB	2.47	0.45
4:N:3:DC:H2''	4:N:4:DG:C8	2.51	0.45
1:P:508:GLY:HA2	1:P:513:ASN:ND2	2.31	0.45
1:F:296:TYR:HB2	1:F:314:ILE:HG13	1.99	0.45
1:K:284:ASN:ND2	1:K:575:TRP:CE3	2.85	0.45
2:Q:1:DC:H2'	2:Q:2:DG:C8	2.52	0.45
1:F:253:ASN:OD1	1:F:292:PRO:HA	2.17	0.45
1:F:489:LEU:HD21	1:F:491:ILE:HD11	1.98	0.45
1:A:403:ALA:HA	1:A:406:PHE:CE1	2.51	0.45
1:F:370:THR:OG1	1:F:373:GLN:HG3	2.16	0.45
1:A:247:GLN:C	1:A:249:ALA:H	2.20	0.45
1:K:569:GLU:O	1:K:572:GLU:HG2	2.17	0.45
1:F:536:VAL:HG12	1:F:537:VAL:N	2.32	0.45
1:A:438:ARG:HG3	1:A:439:SER:N	2.30	0.44
1:K:344:ALA:HA	1:K:373:GLN:HE21	1.82	0.44
1:K:356:GLY:O	1:K:358:ARG:HG2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:431:LEU:HD23	1:P:432:ILE:N	2.32	0.44
1:P:462:VAL:HB	1:P:474:LEU:HB2	2.00	0.44
1:K:492:ILE:HD13	1:K:506:PHE:CZ	2.51	0.44
1:A:279:TYR:O	1:A:283:ILE:HG13	2.17	0.44
1:A:431:LEU:HD23	1:A:431:LEU:C	2.37	0.44
1:K:419:ARG:NH1	1:K:507:THR:HG21	2.32	0.44
1:K:498:GLU:HG2	1:K:530:HIS:O	2.18	0.44
1:P:251:ASN:OD1	1:P:287:LYS:HA	2.17	0.44
1:F:389:ARG:HG3	1:F:389:ARG:NH1	2.32	0.44
1:F:521:LYS:HG3	1:F:538:ARG:NH2	2.32	0.44
1:K:363:ILE:HA	1:K:367:ALA:HB2	2.00	0.44
1:P:378:LYS:NZ	1:P:379:HIS:NE2	2.63	0.44
1:P:569:GLU:HA	1:P:570:PRO:HD3	1.88	0.44
1:F:293:VAL:HA	1:F:298:GLU:OE1	2.18	0.44
1:K:304:GLY:O	4:N:2:DC:H4'	2.18	0.44
1:K:346:THR:HG22	1:K:350:GLN:NE2	2.24	0.44
1:P:363:ILE:C	1:P:365:SER:H	2.20	0.44
2:Q:1:DC:N4	4:S:3:DC:H42	2.16	0.44
1:A:452:ARG:NH2	1:A:465:GLU:OE2	2.51	0.43
1:F:371:THR:HG23	1:F:372:GLN:N	2.33	0.43
1:P:296:TYR:HB2	1:P:314:ILE:HG13	2.00	0.43
1:P:540:THR:HG22	1:P:541:HIS:N	2.34	0.43
1:F:296:TYR:CA	1:F:314:ILE:HD11	2.48	0.43
2:G:4:DC:H2''	2:G:5:DA:H2	1.84	0.43
1:F:440:HIS:NE2	1:F:495:PRO:HG3	2.33	0.43
1:K:337:LEU:HG	1:K:360:LEU:HD21	1.99	0.43
1:F:325:LEU:HD23	1:F:328:ILE:HD11	2.00	0.43
2:G:10:DC:C6	2:G:11:DT:H72	2.54	0.43
1:A:329:SER:C	1:A:331:SER:N	2.71	0.43
1:K:387:MET:HE2	1:K:487:ARG:HD2	2.00	0.43
1:P:316:ILE:HD11	1:P:322:LEU:HD22	2.01	0.43
1:P:516:MET:CE	1:P:565:LEU:HD22	2.48	0.43
1:P:284:ASN:HB3	1:P:575:TRP:NE1	2.34	0.43
1:F:419:ARG:C	1:F:421:GLY:H	2.22	0.43
1:K:532:LEU:HG	1:K:551:LEU:HD12	1.99	0.43
1:K:465:GLU:OE1	1:K:472:LYS:HE2	2.19	0.43
1:F:467:ASN:OD1	1:F:469:GLN:N	2.49	0.43
1:P:516:MET:HE3	1:P:565:LEU:HD22	2.01	0.43
2:Q:11:DT:H2''	2:Q:12:DG:H8	1.83	0.43
1:F:261:GLU:HG3	1:F:283:ILE:HD13	2.01	0.42
1:F:271:GLY:O	1:F:273:LYS:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:PRO:C	1:A:437:GLY:H	2.23	0.42
4:I:1:DG:H2''	4:I:2:DC:H5'	2.01	0.42
1:K:363:ILE:CG2	1:K:369:LEU:HD21	2.49	0.42
1:K:567:TYR:HE1	1:K:569:GLU:OE1	2.02	0.42
1:A:462:VAL:HG21	1:A:474:LEU:HD12	2.01	0.42
1:F:539:ASN:OD1	1:F:543:ALA:HB3	2.19	0.42
1:A:253:ASN:OD1	1:A:292:PRO:HA	2.18	0.42
1:A:328:ILE:O	1:A:329:SER:C	2.57	0.42
1:K:370:THR:O	1:K:371:THR:C	2.58	0.42
1:P:563:LEU:HB3	1:P:565:LEU:HD13	2.01	0.42
1:A:419:ARG:HD3	1:A:507:THR:OG1	2.18	0.42
1:P:271:GLY:CA	1:P:346:THR:HG21	2.49	0.42
1:K:388:PRO:O	1:K:389:ARG:C	2.58	0.42
1:P:278:GLY:HA3	4:S:1:DG:H1'	2.01	0.42
1:F:432:ILE:HB	1:F:493:VAL:HG22	2.01	0.42
1:K:283:ILE:HG22	1:K:287:LYS:HZ3	1.85	0.42
1:P:471:GLN:O	1:P:492:ILE:HA	2.19	0.42
1:A:334:VAL:O	1:A:337:LEU:HB3	2.20	0.42
1:K:353:TYR:C	1:K:355:GLN:H	2.23	0.42
1:P:435:PRO:C	1:P:437:GLY:H	2.22	0.42
2:G:2:DG:H2''	2:G:3:DG:C8	2.55	0.41
1:P:261:GLU:O	1:P:265:LYS:HG3	2.20	0.41
1:K:334:VAL:HG21	1:K:358:ARG:HD2	2.02	0.41
1:K:337:LEU:HD21	1:K:360:LEU:HG	2.02	0.41
1:P:364:ARG:HG2	1:P:364:ARG:HH11	1.86	0.41
1:F:251:ASN:ND2	1:F:254:LEU:CA	2.83	0.41
1:K:521:LYS:C	1:K:523:LYS:H	2.23	0.41
1:P:470:GLN:CG	1:P:494:VAL:HG12	2.45	0.41
1:F:432:ILE:O	1:F:493:VAL:HA	2.20	0.41
2:G:9:DA:H2''	2:G:10:DC:H5'	2.02	0.41
1:K:325:LEU:HD23	1:K:328:ILE:HD11	2.01	0.41
1:K:342:TRP:CD2	1:K:461:LEU:HD13	2.56	0.41
1:K:479:LEU:HA	1:K:480:PRO:HD3	1.93	0.41
1:P:523:LYS:HE3	1:P:563:LEU:O	2.19	0.41
1:F:339:SER:C	1:F:341:ILE:H	2.24	0.41
1:K:420:ARG:O	1:K:571:ALA:HA	2.20	0.41
1:P:468:GLY:HA3	1:P:530:HIS:CE1	2.56	0.41
1:P:561:ARG:HG2	1:P:561:ARG:HH11	1.86	0.41
1:K:363:ILE:O	1:K:367:ALA:HB3	2.21	0.41
1:P:534:THR:OG1	1:P:535:ALA:N	2.53	0.41
1:A:473:TYR:O	1:A:474:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:434:HIS:ND1	1:F:435:PRO:HD2	2.36	0.41
1:K:387:MET:CE	1:K:487:ARG:HB3	2.49	0.41
1:P:315:GLU:OE2	1:P:322:LEU:HD12	2.21	0.41
1:P:407:ASN:HB3	1:P:410:LEU:HG	2.03	0.41
1:P:296:TYR:N	1:P:314:ILE:HD11	2.36	0.41
1:A:304:GLY:O	4:D:2:DC:H4'	2.21	0.40
1:K:261:GLU:CG	1:K:283:ILE:HD13	2.51	0.40
5:K:703:D3T:O4	3:M:6:DT:H2''	2.21	0.40
1:P:495:PRO:C	1:P:497:SER:N	2.75	0.40
1:P:503:LEU:HG	1:P:556:GLU:OE1	2.21	0.40
1:P:414:ALA:O	1:P:419:ARG:HB2	2.20	0.40
1:A:519:LEU:HD11	1:A:523:LYS:HE3	2.02	0.40
1:K:251:ASN:HD22	1:K:254:LEU:HA	1.86	0.40
1:P:387:MET:HB2	1:P:391:GLU:OE1	2.21	0.40
1:K:453:GLN:HA	1:K:453:GLN:NE2	2.37	0.40
1:P:569:GLU:O	1:P:571:ALA:N	2.55	0.40
1:A:444:PHE:CZ	1:A:493:VAL:HG23	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	328/335 (98%)	298 (91%)	25 (8%)	5 (2%)	10	42
1	F	327/335 (98%)	293 (90%)	30 (9%)	4 (1%)	13	48
1	K	325/335 (97%)	285 (88%)	35 (11%)	5 (2%)	10	42
1	P	325/335 (97%)	276 (85%)	43 (13%)	6 (2%)	8	37
All	All	1305/1340 (97%)	1152 (88%)	133 (10%)	20 (2%)	10	42

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	LYS
1	A	407	ASN
1	F	407	ASN
1	F	547	PRO
1	K	540	THR
1	K	545	VAL
1	P	545	VAL
1	F	535	ALA
1	F	543	ALA
1	K	539	ASN
1	P	537	VAL
1	A	539	ASN
1	A	438	ARG
1	K	407	ASN
1	P	540	THR
1	P	570	PRO
1	P	290	HIS
1	P	323	ARG
1	A	437	GLY
1	K	462	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	253/277 (91%)	250 (99%)	3 (1%)	71	90
1	F	256/277 (92%)	255 (100%)	1 (0%)	91	97
1	K	255/277 (92%)	253 (99%)	2 (1%)	81	93
1	P	248/277 (90%)	248 (100%)	0	100	100
All	All	1012/1108 (91%)	1006 (99%)	6 (1%)	86	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
1	A	466	GLU

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Mol	Chain	Res	Type
1	A	506	PHE
1	F	506	PHE
1	K	460	ASP
1	K	469	GLN

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

Mol	Chain	Res	Type
1	A	340	ASN
1	A	350	GLN
1	A	354	GLN
1	A	400	GLN
1	F	400	GLN
1	F	464	GLN
1	F	470	GLN
1	F	471	GLN
1	K	284	ASN
1	K	340	ASN
1	K	350	GLN
1	K	355	GLN
1	K	373	GLN
1	K	400	GLN
1	P	340	ASN
1	P	350	GLN
1	P	354	GLN
1	P	355	GLN
1	P	400	GLN
1	P	404	GLN
1	P	464	GLN
1	P	469	GLN
1	P	470	GLN
1	P	513	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	D3T	K	703	7,6	22,29,29	1.36	2 (9%)	25,45,45	3.13	2 (8%)
5	D3T	F	702	6	22,29,29	1.33	2 (9%)	25,45,45	3.03	1 (4%)
5	D3T	A	701	6	22,29,29	1.34	2 (9%)	25,45,45	3.02	1 (4%)
5	D3T	P	704	7,6	22,29,29	1.36	2 (9%)	25,45,45	3.09	1 (4%)

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	D3T	K	703	7,6	-	7/19/31/31	0/2/2/2
5	D3T	F	702	6	-	1/19/31/31	0/2/2/2
5	D3T	A	701	6	-	3/19/31/31	0/2/2/2
5	D3T	P	704	7,6	-	9/19/31/31	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	703	D3T	C4-N3	4.45	1.40	1.33
5	P	704	D3T	C4-N3	4.31	1.40	1.33
5	A	701	D3T	C4-N3	4.28	1.40	1.33
5	F	702	D3T	C4-N3	4.20	1.40	1.33
5	P	704	D3T	C4-C5	2.82	1.47	1.41
5	F	702	D3T	C4-C5	2.73	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	D3T	C4-C5	2.65	1.47	1.41
5	K	703	D3T	C4-C5	2.63	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	703	D3T	C4-N3-C2	14.63	127.49	115.14
5	P	704	D3T	C4-N3-C2	14.60	127.47	115.14
5	F	702	D3T	C4-N3-C2	14.46	127.35	115.14
5	A	701	D3T	C4-N3-C2	14.45	127.34	115.14
5	K	703	D3T	C4'-O4'-C1'	2.36	112.04	109.81

There are no chirality outliers.

All (20) torsion outliers are listed below:

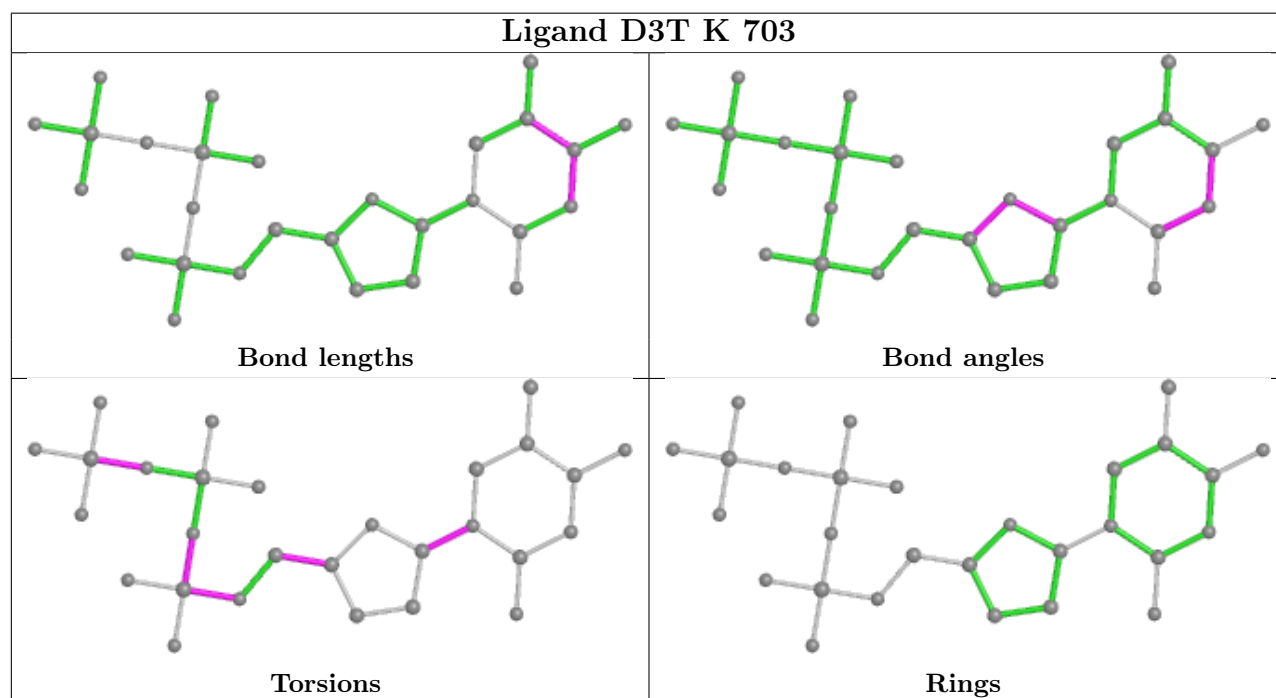
Mol	Chain	Res	Type	Atoms
5	A	701	D3T	PB-O3B-PG-O2G
5	K	703	D3T	C5'-O5'-PA-O1A
5	K	703	D3T	O4'-C1'-N1-C6
5	P	704	D3T	C5'-O5'-PA-O2A
5	P	704	D3T	C5'-O5'-PA-O3A
5	P	704	D3T	O4'-C1'-N1-C6
5	K	703	D3T	O4'-C4'-C5'-O5'
5	K	703	D3T	C5'-O5'-PA-O3A
5	A	701	D3T	PB-O3A-PA-O1A
5	F	702	D3T	PB-O3A-PA-O1A
5	K	703	D3T	PB-O3A-PA-O1A
5	P	704	D3T	PB-O3A-PA-O1A
5	P	704	D3T	C5'-O5'-PA-O1A
5	P	704	D3T	O4'-C4'-C5'-O5'
5	K	703	D3T	C3'-C4'-C5'-O5'
5	P	704	D3T	C3'-C4'-C5'-O5'
5	A	701	D3T	PB-O3B-PG-O3G
5	K	703	D3T	PB-O3B-PG-O2G
5	P	704	D3T	PG-O3B-PB-O1B
5	P	704	D3T	PG-O3B-PB-O2B

There are no ring outliers.

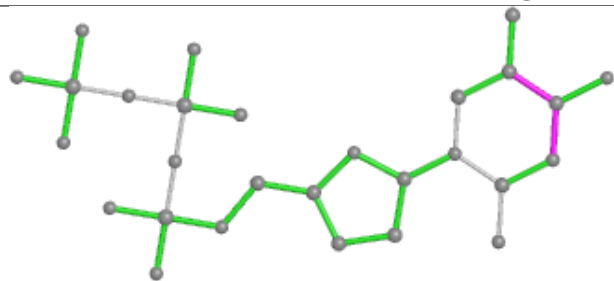
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	703	D3T	1	0

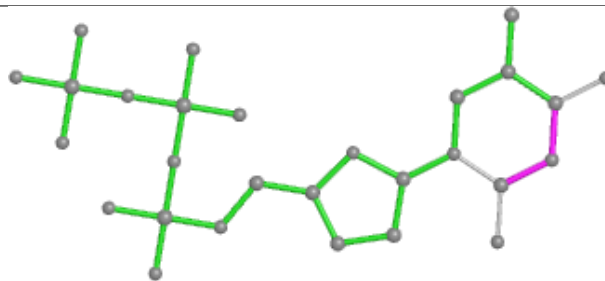
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



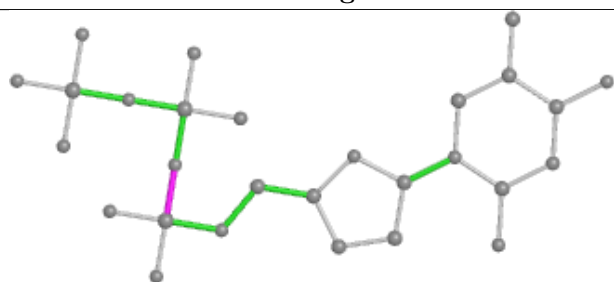
## Ligand D3T F 702



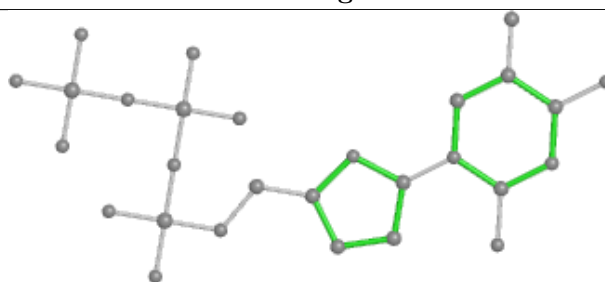
Bond lengths



Bond angles

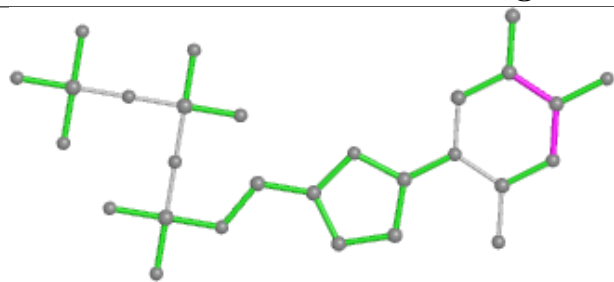


Torsions

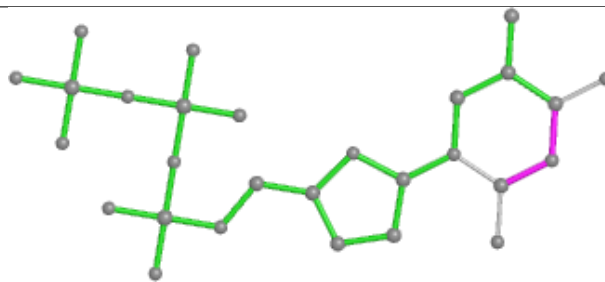


Rings

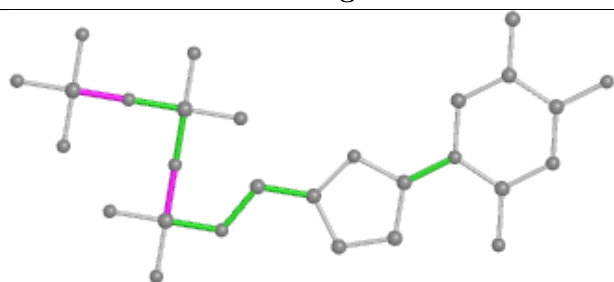
## Ligand D3T A 701



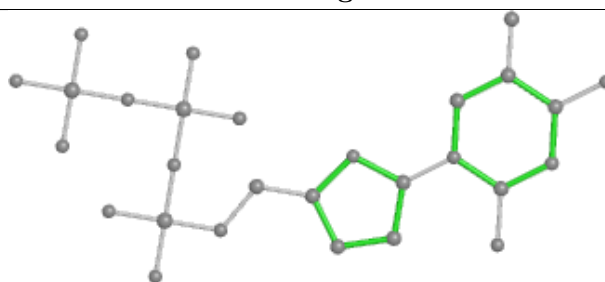
Bond lengths



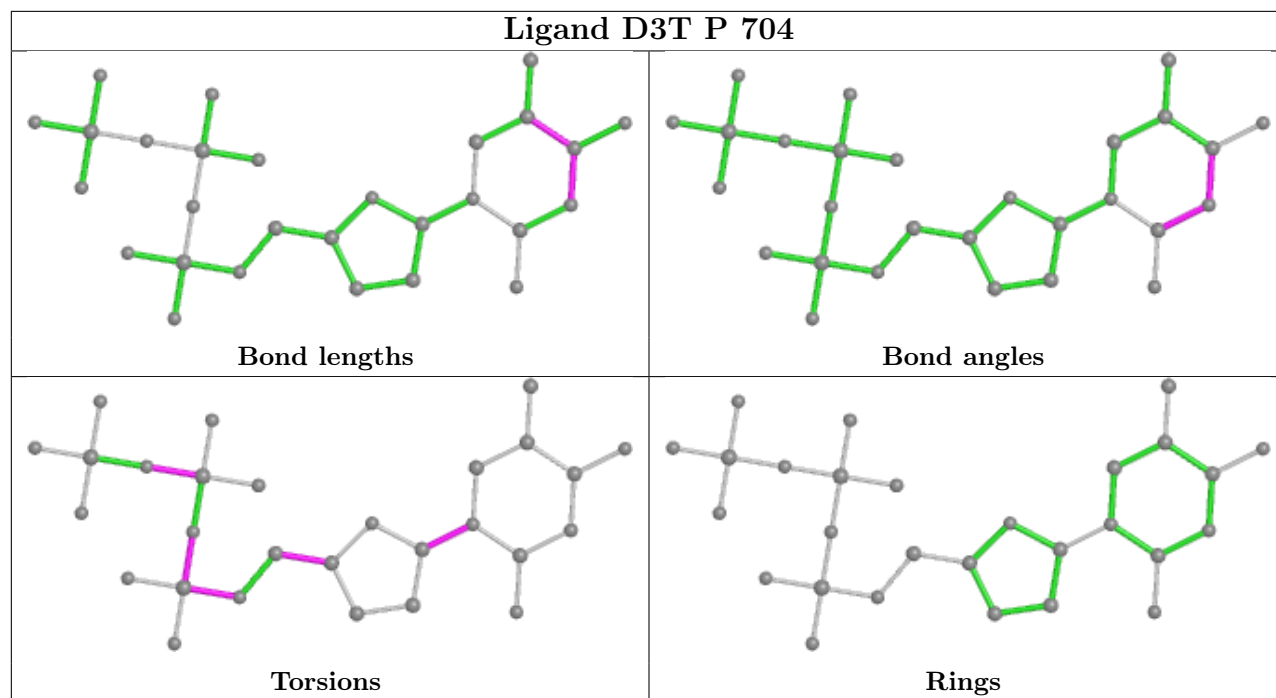
Bond angles



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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	330/335 (98%)	-0.34	3 (0%) 84 63	55, 78, 112, 130	0
1	F	329/335 (98%)	-0.33	2 (0%) 89 72	58, 83, 117, 135	0
1	K	327/335 (97%)	-0.39	0 100 100	59, 83, 115, 136	0
1	P	327/335 (97%)	-0.27	1 (0%) 94 84	77, 103, 120, 141	0
2	B	12/12 (100%)	-0.54	0 100 100	84, 90, 110, 114	0
2	G	12/12 (100%)	-0.64	0 100 100	75, 86, 99, 99	0
2	L	12/12 (100%)	-0.59	0 100 100	67, 71, 77, 79	0
2	Q	12/12 (100%)	-0.64	0 100 100	74, 79, 94, 103	0
3	C	6/6 (100%)	-0.82	0 100 100	77, 85, 104, 109	0
3	H	6/6 (100%)	-0.68	0 100 100	75, 79, 96, 98	0
3	M	6/6 (100%)	-0.67	0 100 100	69, 75, 87, 90	0
3	R	6/6 (100%)	-0.70	0 100 100	78, 83, 90, 96	0
4	D	4/4 (100%)	-0.68	0 100 100	80, 85, 98, 99	0
4	I	4/4 (100%)	-0.65	0 100 100	78, 80, 81, 81	0
4	N	4/4 (100%)	-0.88	0 100 100	80, 83, 86, 87	0
4	S	4/4 (100%)	-0.64	0 100 100	80, 83, 93, 104	0
All	All	1401/1428 (98%)	-0.35	6 (0%) 92 79	55, 87, 118, 141	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	THR	2.5
1	A	539	ASN	2.3
1	P	479	LEU	2.3
1	A	541	HIS	2.3
1	F	544	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	575	TRP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

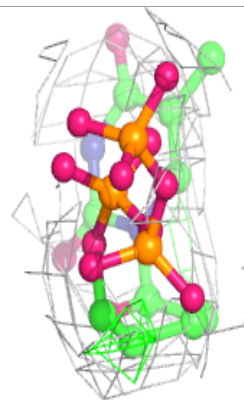
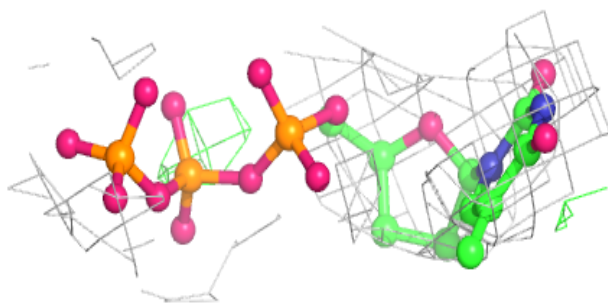
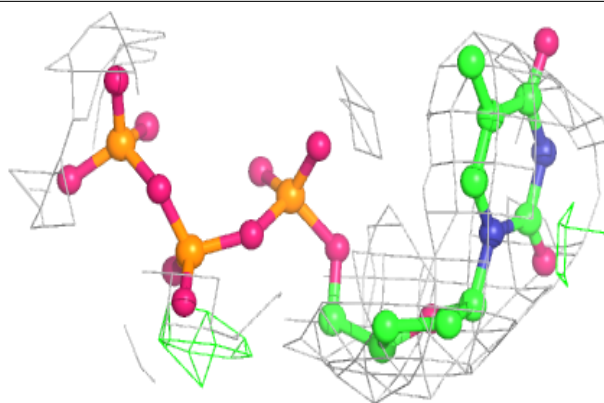
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	NA	K	807	1/1	0.69	0.09	83,83,83,83	0
7	NA	P	809	1/1	0.81	0.12	90,90,90,90	0
7	NA	F	806	1/1	0.82	0.11	97,97,97,97	0
7	NA	K	808	1/1	0.87	0.20	64,64,64,64	0
7	NA	P	810	1/1	0.90	0.09	69,69,69,69	0
6	MG	A	801	1/1	0.96	0.16	68,68,68,68	0
5	D3T	P	704	28/28	0.96	0.19	98,111,128,130	0
5	D3T	A	701	28/28	0.97	0.21	58,64,70,72	0
5	D3T	F	702	28/28	0.97	0.20	59,64,68,70	0
6	MG	K	803	1/1	0.97	0.08	62,62,62,62	0
5	D3T	K	703	28/28	0.97	0.17	76,86,99,101	0
6	MG	P	804	1/1	0.98	0.14	76,76,76,76	0
6	MG	F	802	1/1	0.98	0.13	49,49,49,49	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.

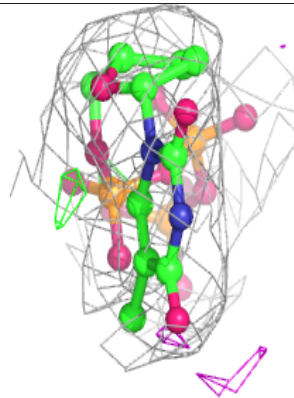
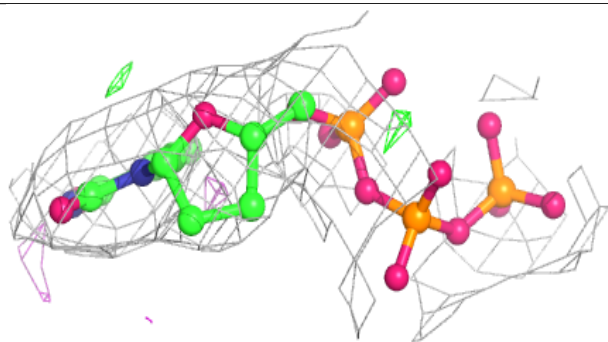
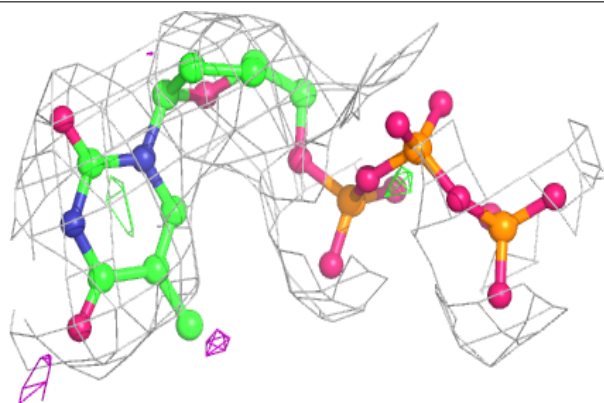


**Electron density around D3T P 704:**

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

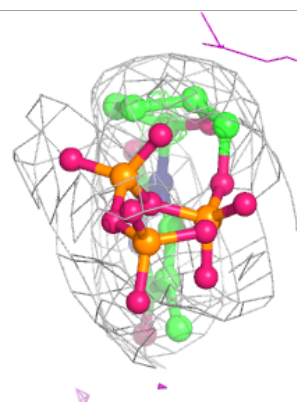
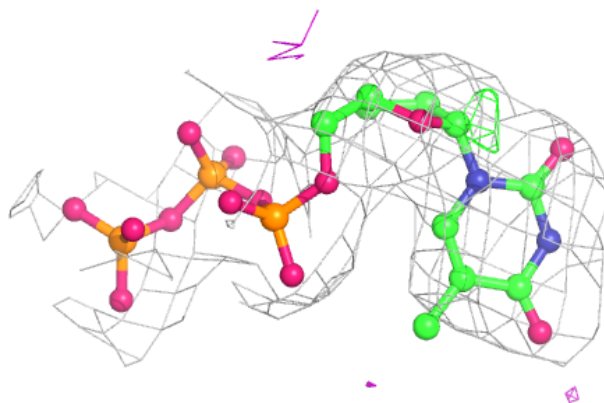
**Electron density around D3T A 701:**

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

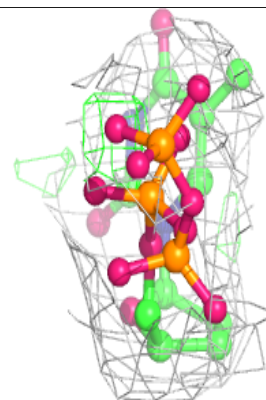
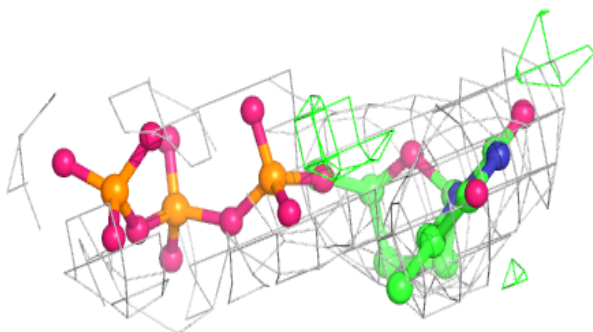
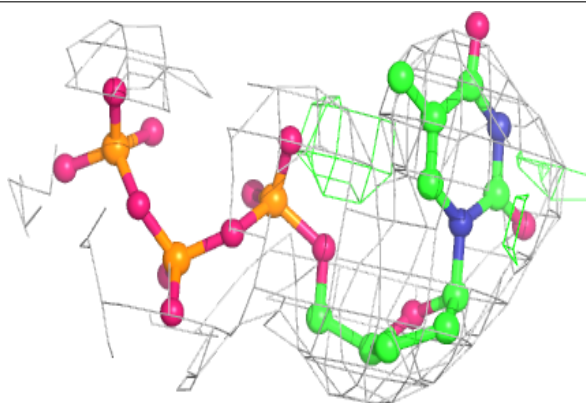


**Electron density around D3T F 702:**

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

**Electron density around D3T K 703:**

$2mF_o - DF_c$  (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.