



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:03 AM BST

PDB ID : 3V6H  
Title : Replication of N2,3-Ethenoguanine by DNA Polymerases  
Authors : Zhao, L.  
Deposited on : 2011-12-19  
Resolution : 2.30 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 : 2.13.1  
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) : 2.13.1

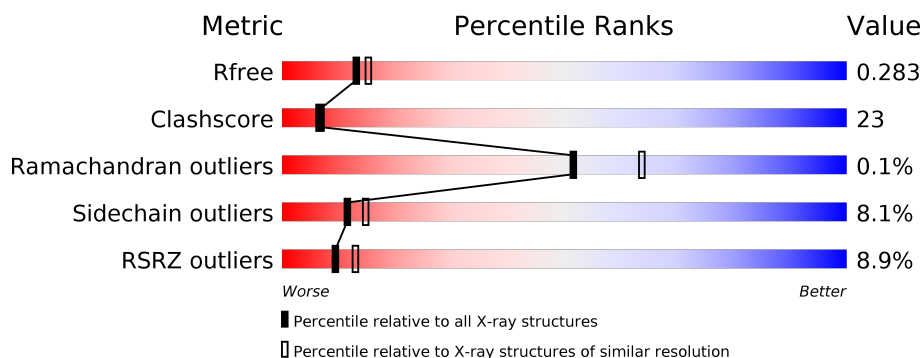
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	C	18	<div> <div>11%</div> <div> <div>17%</div> <div>61%</div> <div>17%</div> <div>6%</div> </div> </div>
1	T	18	<div> <div>28%</div> <div> <div>6%</div> <div>50%</div> <div>17%</div> <div>28%</div> </div> </div>
2	D	13	<div> <div>15%</div> <div> <div>31%</div> <div>38%</div> <div>23%</div> <div>8%</div> </div> </div>
2	P	13	<div> <div>38%</div> <div> <div>38%</div> <div>46%</div> <div>15%</div> </div> </div>
3	A	348	<div> <div>2%</div> <div> <div>80%</div> <div>16%</div> <div>2%</div> </div> </div>
3	B	348	<div> <div>12%</div> <div> <div>74%</div> <div>19%</div> <div>5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DOC	P	13	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6867 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 DNA chain called DNA (5'-D(\*TP\*CP\*AP\*CP\*(EFG)P\*GP\*AP\*AP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	T	13	Total	C	F	N	O	P	0	0	0
			263	126	1	44	79	13			
1	C	17	Total	C	F	N	O	P	0	0	0
			339	164	1	57	101	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	P	0	0	0
			228	109	47	62	10			
2	D	12	Total	C	N	O	P	0	0	0
			250	119	52	68	11			

- Molecule 3 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	343	Total	C	N	O	S	0	0	0
			2762	1771	476	508	7			
3	B	342	Total	C	N	O	S	0	0	0
			2752	1765	473	507	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-4	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-3	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-2	HIS	-	EXPRESSION TAG	UNP Q97W02
A	-1	HIS	-	EXPRESSION TAG	UNP Q97W02
A	0	HIS	-	EXPRESSION TAG	UNP Q97W02

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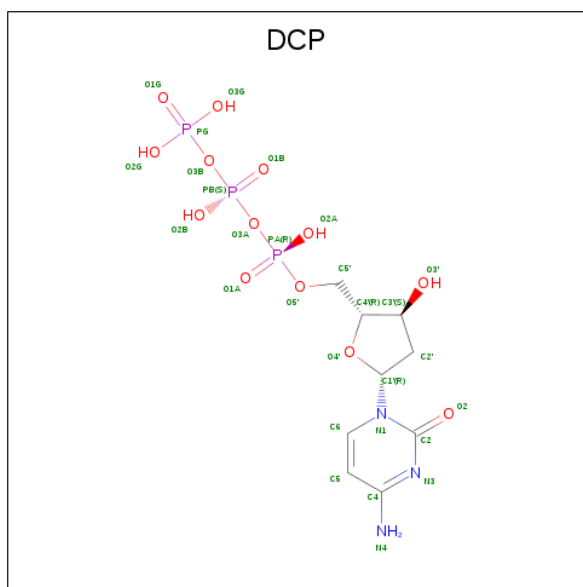
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-4	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-3	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-2	HIS	-	EXPRESSION TAG	UNP Q97W02
B	-1	HIS	-	EXPRESSION TAG	UNP Q97W02
B	0	HIS	-	EXPRESSION TAG	UNP Q97W02

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	Mg 2	0	0
6	A	2	Total 2	Mg 2	0	0

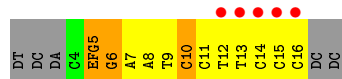
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	T	8	Total 8	O 8	0	0
7	P	4	Total 4	O 4	0	0
7	C	15	Total 15	O 15	0	0
7	D	7	Total 7	O 7	0	0
7	A	115	Total 115	O 115	0	0
7	B	61	Total 61	O 61	0	0

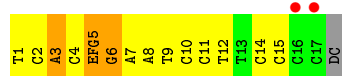
### 3 Residue-property plots [i](#)

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

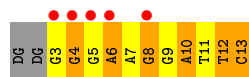
- Molecule 1: DNA (5'-D(\*TP\*CP\*AP\*CP\*(EFG)P\*GP\*AP\*AP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3')



- Molecule 1: DNA (5'-D(\*TP\*CP\*AP\*CP\*(EFG)P\*GP\*AP\*AP\*TP\*CP\*CP\*TP\*TP\*CP\*CP\*CP\*CP\*C)-3')



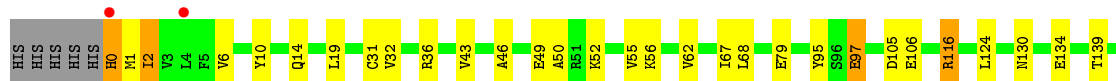
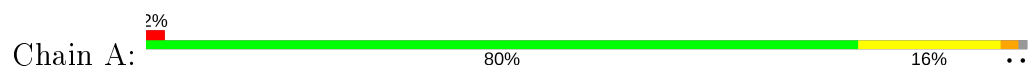
- Molecule 2: DNA (5'-D(\*GP\*G\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*TP\*TP\*(DOC))-3')

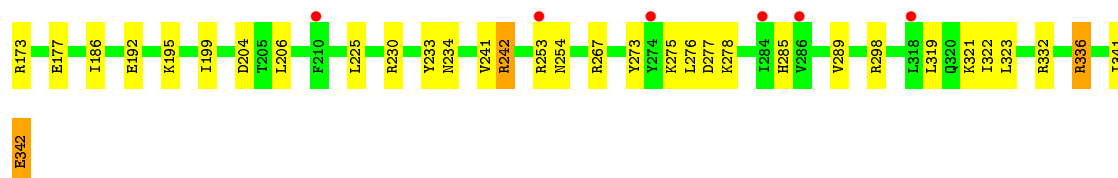


- Molecule 2: DNA (5'-D(\*GP\*G\*GP\*GP\*GP\*AP\*AP\*GP\*GP\*AP\*TP\*TP\*(DOC))-3')

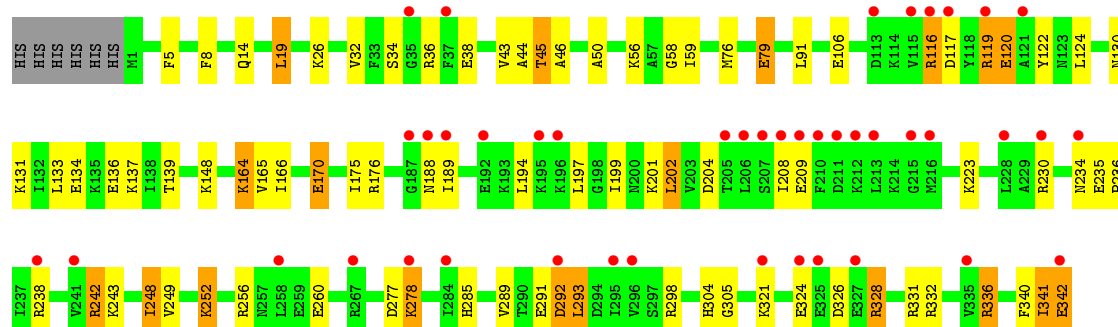
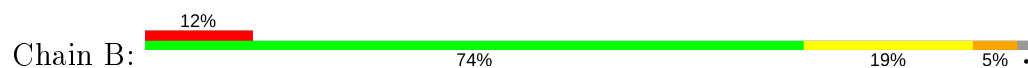


- Molecule 3: DNA polymerase IV





• Molecule 3: DNA polymerase IV





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.53Å 111.27Å 98.94Å 90.00° 102.68° 90.00°	Depositor
Resolution (Å)	27.80 – 2.30 29.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (27.80-2.30) 98.1 (29.80-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.215 , 0.267 0.230 , 0.283	Depositor DCC
$R_{free}$ test set	2446 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6867	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: DOC, MG, CA, DCP, EFG

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	C	0.75	2/348 (0.6%)	1.09	3/530 (0.6%)
1	T	0.36	0/263	0.98	2/399 (0.5%)
2	D	0.55	1/262 (0.4%)	1.05	3/405 (0.7%)
2	P	1.23	3/237 (1.3%)	1.28	5/366 (1.4%)
3	A	0.42	0/2802	0.60	0/3763
3	B	0.36	0/2791	0.57	0/3748
All	All	0.48	6/6703 (0.1%)	0.71	13/9211 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	8	DG	O3'-P	-12.50	1.46	1.61
2	P	4	DG	O3'-P	9.41	1.72	1.61
1	C	1	DT	O3'-P	-6.91	1.52	1.61
1	C	3	DA	O3'-P	-6.88	1.52	1.61
2	D	11	DT	O3'-P	6.27	1.68	1.61
2	P	6	DA	O3'-P	-5.03	1.55	1.61

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	DC	P-O3'-C3'	7.40	128.58	119.70
2	D	11	DT	P-O3'-C3'	7.25	128.40	119.70
1	C	6	DG	C1'-O4'-C4'	-6.91	103.19	110.10
2	D	3	DG	P-O3'-C3'	6.20	127.14	119.70
2	P	12	DT	O5'-P-OP1	-5.90	100.39	105.70
1	T	10	DC	P-O3'-C3'	5.84	126.71	119.70
2	P	4	DG	P-O3'-C3'	-5.79	112.75	119.70
2	P	10	DA	P-O3'-C3'	5.58	126.40	119.70
2	P	9	DG	OP1-P-O3'	5.55	117.41	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	DT	O5'-P-OP1	-5.38	100.85	105.70
2	P	4	DG	O3'-P-O5'	5.37	114.19	104.00
1	C	1	DT	P-O3'-C3'	-5.33	113.30	119.70
1	T	6	DG	P-O3'-C3'	5.28	126.03	119.70

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	C	339	0	192	24	0
1	T	263	0	146	76	0
2	D	250	0	136	28	0
2	P	228	0	125	79	0
3	A	2762	0	2902	50	0
3	B	2752	0	2895	71	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	28	0	12	2	0
5	B	28	0	12	4	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	115	0	0	19	0
7	B	61	0	0	19	0
7	C	15	0	0	2	0
7	D	7	0	0	2	0
7	P	4	0	0	0	0
7	T	8	0	0	0	0
All	All	6867	0	6420	298	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 23.

All (298) 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:T:11:DC:H2'	1:T:12:DT:C6	1.42	1.51
1:T:11:DC:C6	1:T:11:DC:H5''	1.59	1.37
1:T:11:DC:H3'	1:T:12:DT:C7	1.54	1.35
2:P:5:DG:H5''	2:P:5:DG:C8	1.68	1.27
2:P:12:DT:H2'	2:P:13:DOC:C5	1.64	1.25
1:T:11:DC:H2'	1:T:12:DT:C5	1.76	1.21
2:P:11:DT:C6	2:P:12:DT:H72	1.79	1.16
3:B:164:LYS:HE3	3:B:165:VAL:O	1.46	1.15
1:T:11:DC:C2'	1:T:12:DT:C6	2.30	1.14
2:P:7:DA:C4	2:P:8:DG:C8	2.35	1.14
2:D:2:DG:C2'	2:D:3:DG:H2'	1.76	1.13
1:T:15:DC:H1'	1:T:16:DC:O5'	1.49	1.11
2:P:13:DOC:H5''	2:P:13:DOC:H6	1.17	1.11
1:T:11:DC:H3'	1:T:12:DT:H73	1.11	1.10
2:P:12:DT:H2'	2:P:13:DOC:H5	1.11	1.09
2:P:13:DOC:H2'	5:B:401:DCP:H1'	1.35	1.08
1:T:11:DC:H6	1:T:11:DC:C5'	1.65	1.08
1:T:11:DC:H2''	1:T:12:DT:OP1	1.36	1.07
1:T:11:DC:C3'	1:T:12:DT:C7	2.32	1.06
2:P:3:DG:H2''	2:P:4:DG:O5'	1.51	1.06
3:A:36:ARG:HH22	3:A:254:ASN:ND2	1.54	1.05
2:P:12:DT:H2''	2:P:13:DOC:H5''	1.28	1.05
1:C:2:DC:O2	1:C:2:DC:H2'	1.54	1.05
1:T:12:DT:H2''	1:T:13:DT:H5'	1.36	1.05
3:B:341:ILE:HA	7:B:505:HOH:O	1.57	1.04
2:P:12:DT:H2''	2:P:13:DOC:H6	1.34	1.03
2:P:12:DT:H2''	2:P:13:DOC:C6	1.86	1.03
1:T:14:DC:H2''	1:T:15:DC:O5'	1.58	1.03
2:D:2:DG:H2'	2:D:3:DG:H2'	1.37	1.03
2:D:2:DG:O3'	2:D:3:DG:H3'	1.60	1.02
1:T:11:DC:H3'	1:T:12:DT:H72	1.42	1.02
2:P:12:DT:C2'	2:P:13:DOC:C5	2.37	1.01
2:P:5:DG:C5'	2:P:5:DG:H8	1.71	1.01
3:B:14:GLN:HE22	3:B:139:THR:H	1.06	1.01
2:P:10:DA:H2'	2:P:11:DT:H71	1.43	1.01
1:T:15:DC:H2''	1:T:16:DC:OP2	1.63	0.99
1:T:11:DC:H6	1:T:11:DC:H5''	0.81	0.98
3:B:248:ILE:HD11	3:B:332:ARG:HB3	1.44	0.97
2:P:12:DT:C2'	2:P:13:DOC:C6	2.42	0.97
3:A:67:ILE:HG13	7:A:609:HOH:O	1.62	0.97
2:P:7:DA:C2	2:P:8:DG:C4	2.53	0.97
1:T:14:DC:H1'	1:T:15:DC:H5''	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:43:VAL:HB	7:B:561:HOH:O	1.63	0.95
2:P:5:DG:H5''	2:P:5:DG:H8	0.80	0.94
2:P:7:DA:N3	2:P:8:DG:C8	2.35	0.94
3:B:242:ARG:HG3	3:B:242:ARG:HH11	1.32	0.93
1:T:8:DA:H2	2:P:11:DT:H3	1.17	0.93
2:P:7:DA:C5	2:P:8:DG:N7	2.36	0.93
2:P:7:DA:C6	2:P:8:DG:C5	2.56	0.92
3:A:319:LEU:HD12	7:A:580:HOH:O	1.70	0.92
2:P:5:DG:C5'	2:P:5:DG:C8	2.50	0.92
2:P:12:DT:H2''	2:P:13:DOC:C5'	2.00	0.90
1:T:11:DC:C6	1:T:11:DC:C5'	2.48	0.89
2:P:7:DA:N1	2:P:8:DG:C5	2.39	0.89
3:B:164:LYS:CE	3:B:165:VAL:O	2.21	0.89
1:T:11:DC:C3'	1:T:12:DT:H73	1.98	0.89
2:D:6:DA:H4'	2:D:7:DA:OP1	1.72	0.89
1:T:11:DC:C3'	1:T:12:DT:H72	1.98	0.88
2:D:2:DG:H2''	2:D:3:DG:H2'	1.53	0.88
3:B:164:LYS:HE2	3:B:166:ILE:HG12	1.54	0.88
2:P:7:DA:H2''	2:P:8:DG:O5'	1.75	0.87
3:A:14:GLN:HE22	3:A:139:THR:H	1.20	0.87
1:T:11:DC:H2'	1:T:12:DT:H6	1.36	0.87
1:T:7:DA:C2	2:P:12:DT:N3	2.43	0.86
1:T:14:DC:H1'	1:T:15:DC:C5'	2.06	0.86
1:T:12:DT:O2	1:T:13:DT:C2	2.30	0.84
3:A:36:ARG:NH2	3:A:254:ASN:ND2	2.26	0.84
3:A:1:MET:C	3:A:2:ILE:HD13	1.97	0.84
2:P:5:DG:H2''	2:P:6:DA:O4'	1.79	0.83
2:P:7:DA:C2	2:P:8:DG:N9	2.47	0.82
1:T:7:DA:H2	2:P:12:DT:H3	1.25	0.82
2:D:6:DA:H2'	2:D:7:DA:C8	2.16	0.81
3:B:201:LYS:HE2	7:B:501:HOH:O	1.82	0.80
1:T:15:DC:C1'	1:T:16:DC:O5'	2.30	0.79
1:T:14:DC:C2'	1:T:15:DC:O5'	2.31	0.79
2:P:7:DA:C6	2:P:8:DG:N7	2.51	0.79
3:A:2:ILE:N	3:A:2:ILE:HD13	1.94	0.79
3:B:201:LYS:CE	7:B:501:HOH:O	2.31	0.79
2:D:2:DG:H2''	2:D:3:DG:C2'	2.13	0.78
1:C:3:DA:H5''	1:C:3:DA:H8	1.48	0.78
7:D:204:HOH:O	3:A:285:HIS:HE1	1.67	0.77
1:C:2:DC:O2	1:C:2:DC:C2'	2.30	0.77
3:A:79:GLU:H	3:A:79:GLU:CD	1.87	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:248:ILE:CD1	3:B:332:ARG:HB3	2.14	0.76
2:P:7:DA:C2	2:P:8:DG:C8	2.72	0.76
1:T:11:DC:C2'	1:T:12:DT:H6	1.90	0.76
1:C:7:DA:C2	2:D:12:DT:N3	2.52	0.76
2:P:13:DOC:H2'	5:B:401:DCP:C1'	2.15	0.75
3:A:275:LYS:HE3	7:A:563:HOH:O	1.85	0.75
3:A:31:CYS:SG	7:A:581:HOH:O	2.43	0.75
2:P:13:DOC:H5''	2:P:13:DOC:C6	2.09	0.75
2:P:13:DOC:H6	2:P:13:DOC:C5'	2.09	0.75
3:B:164:LYS:HE2	3:B:166:ILE:CG1	2.17	0.74
3:B:175:ILE:HG23	7:B:542:HOH:O	1.87	0.74
2:D:2:DG:C2'	2:D:3:DG:C2'	2.61	0.74
3:B:341:ILE:HG22	3:B:342:GLU:H	1.53	0.73
1:T:14:DC:H1'	1:T:15:DC:OP1	1.87	0.73
3:B:166:ILE:HG23	3:B:170:GLU:HB3	1.71	0.73
2:P:11:DT:C6	2:P:12:DT:C7	2.69	0.73
2:P:7:DA:C4	2:P:8:DG:N7	2.57	0.72
1:T:7:DA:H2	2:P:12:DT:C2	2.07	0.72
2:P:3:DG:C2'	2:P:4:DG:O5'	2.35	0.71
1:T:7:DA:H2	2:P:12:DT:N3	1.82	0.71
1:T:11:DC:C2'	1:T:12:DT:C7	2.69	0.71
2:P:13:DOC:C2'	5:B:401:DCP:H1'	2.19	0.71
1:C:7:DA:H2	2:D:12:DT:C2	2.09	0.70
3:B:292:ASP:OD2	3:B:328:ARG:NH1	2.20	0.70
1:T:11:DC:C2'	1:T:12:DT:C5	2.62	0.69
1:C:3:DA:H5''	1:C:3:DA:C8	2.27	0.69
1:C:5:EFG:H1	5:A:401:DCP:HN41	1.41	0.69
2:P:7:DA:C2	2:P:8:DG:C5	2.79	0.69
1:C:5:EFG:H1'	1:C:5:EFG:H10	1.73	0.69
2:P:4:DG:N7	2:P:5:DG:C2	2.62	0.68
2:D:3:DG:P	2:D:3:DG:H3'	2.34	0.68
1:C:7:DA:H2	2:D:12:DT:O2	1.76	0.68
3:A:52:LYS:HE3	7:A:561:HOH:O	1.92	0.68
1:T:14:DC:C1'	1:T:15:DC:C5'	2.71	0.68
3:A:342:GLU:C	7:A:538:HOH:O	2.32	0.67
1:T:13:DT:C6	1:T:14:DC:N4	2.62	0.67
3:A:43:VAL:HA	7:A:581:HOH:O	1.95	0.67
1:T:5:EFG:H1'	1:T:5:EFG:H10	1.76	0.67
2:D:6:DA:C2'	2:D:7:DA:C8	2.77	0.66
3:B:119:ARG:O	3:B:122:TYR:HB3	1.96	0.66
3:B:289:VAL:HB	3:B:332:ARG:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:97:GLU:HA	7:A:569:HOH:O	1.95	0.65
1:T:11:DC:H2'	1:T:12:DT:C7	2.27	0.65
3:A:0:HIS:O	3:A:0:HIS:ND1	2.30	0.65
3:B:59:ILE:N	7:B:561:HOH:O	2.29	0.65
3:B:292:ASP:OD1	3:B:292:ASP:N	2.30	0.65
1:T:14:DC:H2''	1:T:15:DC:C5'	2.26	0.65
3:B:285:HIS:HD2	7:B:523:HOH:O	1.78	0.64
2:P:12:DT:C2'	2:P:13:DOC:H6	2.13	0.64
1:T:14:DC:N4	2:P:5:DG:H22	1.96	0.63
3:B:238:ARG:HG3	3:B:238:ARG:O	1.98	0.63
2:P:12:DT:C2'	2:P:13:DOC:H5''	2.18	0.63
2:P:7:DA:C6	2:P:8:DG:C6	2.87	0.62
3:A:277:ASP:O	3:A:278:LYS:HB2	1.99	0.62
1:T:6:DG:N7	2:P:13:DOC:O2	2.33	0.62
1:T:14:DC:H1'	1:T:15:DC:P	2.40	0.61
3:B:202:LEU:HB2	7:B:535:HOH:O	1.99	0.61
2:P:7:DA:N1	2:P:8:DG:C4	2.66	0.61
3:A:199:ILE:HG23	3:A:204:ASP:HB2	1.82	0.61
2:P:4:DG:C8	2:P:5:DG:C6	2.89	0.61
1:T:15:DC:H1'	1:T:16:DC:C5'	2.31	0.60
3:A:241:VAL:HB	7:A:560:HOH:O	2.01	0.60
3:A:285:HIS:HD2	7:A:550:HOH:O	1.83	0.60
2:D:13:DOC:C5'	7:A:614:HOH:O	2.48	0.60
3:B:164:LYS:HE3	3:B:165:VAL:C	2.20	0.60
1:T:5:EFG:H9	3:B:32:VAL:HG21	1.82	0.60
1:T:9:DT:H2'	1:T:10:DC:C6	2.36	0.60
3:B:130:ASN:O	3:B:134:GLU:HG2	2.02	0.60
2:P:5:DG:H2'	2:P:6:DA:C8	2.37	0.60
3:B:341:ILE:CA	7:B:505:HOH:O	2.32	0.59
2:P:10:DA:H4'	2:P:11:DT:OP1	2.00	0.59
3:A:130:ASN:O	3:A:134:GLU:HG2	2.02	0.59
2:P:12:DT:C2'	2:P:13:DOC:H5	2.04	0.59
3:B:56:LYS:HB2	7:B:546:HOH:O	2.01	0.59
3:B:194:LEU:HB3	3:B:199:ILE:HB	1.86	0.58
3:B:14:GLN:NE2	3:B:139:THR:H	1.90	0.57
1:T:7:DA:H2	2:P:12:DT:O2	1.87	0.57
1:T:11:DC:C2'	1:T:12:DT:OP1	2.30	0.57
1:T:14:DC:N4	2:P:5:DG:N2	2.53	0.57
3:A:49:GLU:HA	3:A:52:LYS:HE2	1.86	0.57
3:B:277:ASP:O	3:B:278:LYS:HD3	2.04	0.57
2:P:11:DT:C5	2:P:12:DT:H72	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:201:LYS:HE3	7:B:501:HOH:O	2.00	0.57
1:T:5:EFG:H4'	3:B:34:SER:HB3	1.86	0.57
3:A:341:ILE:O	3:A:342:GLU:C	2.43	0.56
3:B:148:LYS:HE3	7:B:557:HOH:O	2.05	0.56
3:B:252:LYS:HE3	7:B:503:HOH:O	2.06	0.56
1:C:6:DG:H21	3:A:332:ARG:NH1	2.02	0.56
1:C:7:DA:H2	2:D:12:DT:N3	1.99	0.56
2:P:4:DG:C2'	2:P:5:DG:O5'	2.53	0.56
3:B:14:GLN:HE22	3:B:139:THR:N	1.89	0.55
2:P:7:DA:N3	2:P:8:DG:N9	2.50	0.55
3:B:326:ASP:OD1	3:B:328:ARG:HG3	2.07	0.55
2:P:11:DT:H2''	2:P:12:DT:H6	1.72	0.55
3:B:46:ALA:HB1	3:B:50:ALA:HB3	1.89	0.55
2:D:2:DG:C4	2:D:3:DG:C8	2.95	0.54
3:B:79:GLU:H	3:B:79:GLU:CD	2.09	0.54
1:C:11:DC:H4'	7:A:519:HOH:O	2.07	0.54
3:B:208:ILE:HG13	3:B:209:GLU:H	1.71	0.54
2:P:6:DA:H2''	2:P:7:DA:H8	1.71	0.54
3:B:326:ASP:OD2	3:B:328:ARG:HG3	2.07	0.54
2:D:2:DG:C4	2:D:3:DG:N7	2.76	0.54
3:B:242:ARG:HH11	3:B:242:ARG:CG	2.12	0.54
3:B:58:GLY:N	7:B:561:HOH:O	2.40	0.54
3:B:291:GLU:HG3	3:B:292:ASP:OD1	2.08	0.53
3:B:44:ALA:O	5:B:401:DCP:H2'1	2.09	0.53
2:D:2:DG:C3'	2:D:3:DG:H3'	2.37	0.53
2:D:13:DOC:H5''	7:A:614:HOH:O	2.07	0.53
1:T:14:DC:C1'	1:T:15:DC:P	2.95	0.53
3:A:186:ILE:HD11	3:A:225:LEU:HD21	1.90	0.53
1:T:13:DT:O2	2:P:7:DA:C2	2.62	0.52
3:A:289:VAL:HB	3:A:332:ARG:HB2	1.90	0.52
1:T:11:DC:C2'	1:T:12:DT:H72	2.38	0.52
2:D:2:DG:H2''	2:D:3:DG:C3'	2.39	0.52
1:T:14:DC:C1'	1:T:15:DC:H5''	2.27	0.52
3:B:340:PHE:CD1	3:B:340:PHE:N	2.77	0.52
2:P:4:DG:C8	2:P:5:DG:C5	2.98	0.52
1:T:12:DT:C2'	1:T:13:DT:H5'	2.26	0.51
2:P:11:DT:H2''	2:P:12:DT:C6	2.46	0.51
2:P:11:DT:C2'	2:P:12:DT:C6	2.94	0.51
7:D:204:HOH:O	3:A:285:HIS:CE1	2.51	0.51
1:C:5:EFG:C9	3:A:32:VAL:HG21	2.40	0.51
1:T:14:DC:C2'	1:T:15:DC:C5'	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:DA:H2''	2:P:7:DA:C8	2.46	0.51
1:T:15:DC:C6	1:T:16:DC:H5'	2.46	0.50
1:T:8:DA:P	3:B:336:ARG:HH22	2.35	0.50
1:C:3:DA:N6	1:C:4:DC:N4	2.60	0.50
1:T:15:DC:P	1:T:15:DC:H3'	2.52	0.50
3:B:199:ILE:HG23	3:B:204:ASP:HB2	1.93	0.49
3:A:242:ARG:NH1	7:A:597:HOH:O	2.46	0.49
3:B:292:ASP:O	3:B:293:LEU:HB2	2.12	0.49
2:P:4:DG:H2'	2:P:5:DG:C8	2.48	0.49
1:T:13:DT:C5	1:T:14:DC:N4	2.81	0.49
1:C:7:DA:C2	2:D:12:DT:C2	2.95	0.49
2:P:11:DT:H2'	2:P:12:DT:C7	2.43	0.49
1:T:11:DC:C4'	1:T:11:DC:C6	2.95	0.49
1:T:12:DT:OP1	1:T:12:DT:O4'	2.30	0.49
1:T:15:DC:C2'	1:T:16:DC:O5'	2.60	0.49
3:A:67:ILE:CG1	7:A:609:HOH:O	2.40	0.49
3:B:331:ARG:HG2	3:B:332:ARG:HG3	1.95	0.49
2:P:10:DA:H2'	2:P:11:DT:C7	2.29	0.48
1:T:5:EFG:C10	3:B:32:VAL:HG21	2.44	0.48
3:A:273:TYR:HA	3:A:276:LEU:HD12	1.93	0.48
3:B:136:GLU:O	3:B:137:LYS:CB	2.62	0.48
2:D:12:DT:H2''	2:D:13:DOC:H6	1.96	0.48
3:A:322:ILE:HB	7:A:580:HOH:O	2.12	0.48
3:B:298:ARG:NH1	3:B:321:LYS:HG2	2.29	0.48
2:P:7:DA:N6	2:P:8:DG:C6	2.81	0.48
1:T:11:DC:O2	2:P:8:DG:N2	2.34	0.48
1:T:14:DC:C1'	1:T:15:DC:OP1	2.59	0.47
3:B:326:ASP:CG	3:B:328:ARG:HG3	2.35	0.47
3:B:136:GLU:O	3:B:137:LYS:HB2	2.15	0.47
2:P:3:DG:N2	2:P:4:DG:C2	2.82	0.47
3:B:248:ILE:HD13	3:B:249:VAL:N	2.29	0.47
3:B:304:HIS:HD2	3:B:305:GLY:O	1.98	0.47
1:C:6:DG:H5'	3:A:32:VAL:HG11	1.97	0.47
3:B:5:PHE:CZ	3:B:106:GLU:HG2	2.50	0.47
3:B:8:PHE:HZ	7:B:522:HOH:O	1.97	0.47
1:C:9:DT:H2''	1:C:10:DC:H5'	1.95	0.46
2:P:7:DA:N1	2:P:8:DG:C6	2.82	0.46
1:T:15:DC:C1'	1:T:16:DC:C5'	2.93	0.46
1:T:13:DT:H2''	1:T:14:DC:C2	2.49	0.46
1:C:12:DT:H2'	7:C:111:HOH:O	2.15	0.46
2:P:4:DG:N7	2:P:5:DG:N1	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:5:EFG:H1'	1:T:5:EFG:C9	2.43	0.46
3:A:233:TYR:CD1	3:A:233:TYR:C	2.89	0.46
3:B:116:ARG:HG2	3:B:120:GLU:OE1	2.16	0.45
3:B:341:ILE:C	7:B:505:HOH:O	2.54	0.45
2:P:11:DT:C2'	2:P:12:DT:H6	2.29	0.45
3:A:298:ARG:HD2	3:A:321:LYS:HD3	1.99	0.45
3:B:235:GLU:HG3	3:B:236:PRO:HD2	1.99	0.45
1:C:5:EFG:H10	3:A:32:VAL:HG21	1.99	0.44
3:B:260:GLU:HA	7:B:532:HOH:O	2.18	0.44
2:P:3:DG:H1'	2:P:4:DG:O4'	2.17	0.44
1:C:5:EFG:C9	1:C:5:EFG:H1'	2.42	0.44
1:T:14:DC:C4	2:P:5:DG:N2	2.85	0.44
1:T:15:DC:H3'	1:T:15:DC:OP2	2.18	0.44
3:A:1:MET:SD	3:A:234:ASN:ND2	2.88	0.44
3:A:55:VAL:HG21	3:A:68:LEU:HD12	2.00	0.44
3:B:242:ARG:NH1	3:B:242:ARG:CG	2.77	0.43
1:T:15:DC:H1'	1:T:16:DC:P	2.56	0.43
1:T:15:DC:C2'	1:T:16:DC:OP2	2.46	0.43
3:B:117:ASP:OD1	3:B:119:ARG:HB2	2.18	0.43
1:T:14:DC:H41	2:P:5:DG:H22	1.67	0.43
1:T:11:DC:C5'	1:T:12:DT:H72	2.49	0.43
1:T:13:DT:H6	1:T:13:DT:H2'	1.69	0.43
3:A:46:ALA:HB1	3:A:50:ALA:HB3	2.00	0.43
3:A:242:ARG:HH11	3:A:242:ARG:CG	2.32	0.42
3:A:95:TYR:HD2	3:A:124:LEU:HD11	1.84	0.42
2:D:6:DA:H2''	2:D:7:DA:O5'	2.20	0.42
2:P:10:DA:O3'	3:B:189:ILE:HB	2.19	0.42
1:T:11:DC:C6	1:T:12:DT:H72	2.54	0.42
3:B:45:THR:HG21	7:B:559:HOH:O	2.19	0.42
2:P:7:DA:N6	2:P:8:DG:O6	2.53	0.42
3:A:173:ARG:NH1	3:A:177:GLU:OE1	2.52	0.42
3:B:326:ASP:OD1	3:B:328:ARG:CG	2.67	0.42
7:A:562:HOH:O	3:B:19:LEU:HG	2.20	0.42
2:D:5:DG:C2'	2:D:6:DA:C8	3.02	0.42
1:C:8:DA:P	3:A:336:ARG:HH22	2.43	0.42
3:A:241:VAL:HG13	7:A:592:HOH:O	2.20	0.42
3:B:124:LEU:HD12	7:B:513:HOH:O	2.19	0.42
1:C:10:DC:H1'	7:C:102:HOH:O	2.20	0.42
2:D:13:DOC:H5'	7:A:614:HOH:O	2.15	0.42
1:T:9:DT:OP1	3:B:243:LYS:N	2.38	0.42
1:C:6:DG:H21	3:A:332:ARG:CZ	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:DC:OP2	1:C:15:DC:H2'	2.20	0.41
2:D:2:DG:H2'	2:D:3:DG:H8	1.86	0.41
3:A:2:ILE:HD12	3:A:2:ILE:HA	1.84	0.41
2:D:6:DA:C4'	2:D:7:DA:OP1	2.56	0.41
3:A:10:TYR:HA	5:A:401:DCP:PB	2.61	0.41
3:A:6:VAL:O	3:A:106:GLU:HA	2.21	0.41
3:A:206:LEU:HD21	3:A:230:ARG:HG3	2.02	0.41
2:P:12:DT:C2'	2:P:13:DOC:C5'	2.84	0.40
3:A:116:ARG:HE	3:A:116:ARG:HB2	1.66	0.40
2:D:5:DG:H2''	2:D:6:DA:C8	2.56	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	
3	A	341/348 (98%)	329 (96%)	12 (4%)	0	100	100
3	B	340/348 (98%)	326 (96%)	13 (4%)	1 (0%)	41	50
All	All	681/696 (98%)	655 (96%)	25 (4%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	341	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	302/307 (98%)	286 (95%)	16 (5%)	22	31
3	B	301/307 (98%)	268 (89%)	33 (11%)	6	7
All	All	603/614 (98%)	554 (92%)	49 (8%)	11	15

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	0	HIS
3	A	2	ILE
3	A	19	LEU
3	A	56	LYS
3	A	62	VAL
3	A	97	GLU
3	A	105	ASP
3	A	116	ARG
3	A	192	GLU
3	A	195	LYS
3	A	242	ARG
3	A	253	ARG
3	A	267	ARG
3	A	323	LEU
3	A	336	ARG
3	A	342	GLU
3	B	19	LEU
3	B	26	LYS
3	B	36	ARG
3	B	38	GLU
3	B	45	THR
3	B	76	MET
3	B	79	GLU
3	B	91	LEU
3	B	116	ARG
3	B	119	ARG
3	B	120	GLU
3	B	131	LYS
3	B	133	LEU
3	B	164	LYS
3	B	170	GLU
3	B	176	ARG
3	B	188	ASN

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Mol	Chain	Res	Type
3	B	197	LEU
3	B	202	LEU
3	B	223	LYS
3	B	230	ARG
3	B	234	ASN
3	B	242	ARG
3	B	248	ILE
3	B	252	LYS
3	B	256	ARG
3	B	278	LYS
3	B	292	ASP
3	B	293	LEU
3	B	324	GLU
3	B	328	ARG
3	B	336	ARG
3	B	342	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	14	GLN
3	A	254	ASN
3	A	304	HIS
3	A	320	GLN
3	B	14	GLN
3	B	82	GLN
3	B	188	ASN
3	B	234	ASN
3	B	304	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	DOC	P	13	2	14,19,20	1.26	2 (14%)	13,26,29	2.58	6 (46%)
1	EFG	C	5	1	18,28,29	1.79	4 (22%)	17,42,45	1.90	5 (29%)
1	EFG	T	5	1	18,28,29	1.95	4 (22%)	17,42,45	1.20	1 (5%)
2	DOC	D	13	1,2	14,19,20	1.36	3 (21%)	13,26,29	1.95	4 (30%)

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
2	DOC	P	13	2	-	1/4/18/19	0/2/2/2
1	EFG	C	5	1	-	2/3/25/26	0/4/4/4
1	EFG	T	5	1	-	3/3/25/26	0/4/4/4
2	DOC	D	13	1,2	-	0/4/18/19	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	5	EFG	C6-N1	4.35	1.40	1.33
1	C	5	EFG	O4'-C1'	4.29	1.47	1.41
1	T	5	EFG	O4'-C1'	4.25	1.47	1.41
1	T	5	EFG	C6-C5	-3.56	1.35	1.41
1	C	5	EFG	C6-N1	3.45	1.39	1.33
1	C	5	EFG	C6-C5	-3.32	1.35	1.41
2	D	13	DOC	C2-N3	-3.03	1.32	1.38
2	P	13	DOC	C6-N1	-2.81	1.32	1.35
2	D	13	DOC	C6-N1	-2.54	1.32	1.35
1	C	5	EFG	C5-C4	-2.34	1.34	1.40
1	T	5	EFG	C5-C4	-2.31	1.34	1.40
2	D	13	DOC	C4-N3	-2.17	1.32	1.35
2	P	13	DOC	C2-N3	-2.11	1.34	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	13	DOC	C4'-O4'-C1'	4.94	114.47	109.81
2	P	13	DOC	C2-N3-C4	4.87	121.28	116.34
2	D	13	DOC	C2'-C1'-N1	4.51	120.97	112.48
1	C	5	EFG	F-C2'-C3'	-3.19	102.56	109.22
2	P	13	DOC	C3'-C2'-C1'	2.94	106.18	102.78
2	D	13	DOC	C4'-O4'-C1'	2.91	112.55	109.81
1	C	5	EFG	C3'-C2'-C1'	2.88	106.62	103.13
1	C	5	EFG	C2'-C3'-C4'	2.80	106.02	102.40
1	C	5	EFG	F-C2'-C1'	2.79	114.89	109.08
2	D	13	DOC	C2-N3-C4	2.64	119.02	116.34
1	C	5	EFG	C5-C6-N1	-2.60	119.87	123.43
2	P	13	DOC	N4-C4-N3	2.54	120.51	116.49
2	D	13	DOC	O4'-C4'-C5'	2.50	113.62	109.52
2	P	13	DOC	O4'-C1'-C2'	-2.46	104.00	106.67
2	P	13	DOC	C5-C4-N3	-2.27	119.10	121.72
1	T	5	EFG	C5-C6-N1	-2.22	120.40	123.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	T	5	EFG	O4'-C4'-C5'-O5'
1	T	5	EFG	C3'-C4'-C5'-O5'
1	C	5	EFG	O4'-C4'-C5'-O5'
1	C	5	EFG	C3'-C4'-C5'-O5'
1	T	5	EFG	C4'-C5'-O5'-P
2	P	13	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	13	DOC	19	0
1	C	5	EFG	5	0
1	T	5	EFG	5	0
2	D	13	DOC	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	DCP	B	401	6	23,29,29	0.73	0	30,45,45	1.66	6 (20%)
5	DCP	A	401	6	23,29,29	0.60	0	30,45,45	1.32	3 (10%)

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	DCP	B	401	6	-	4/19/34/34	0/2/2/2
5	DCP	A	401	6	-	3/19/34/34	0/2/2/2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	DCP	C2-N3-C4	4.26	120.66	116.34
5	B	401	DCP	PB-O3B-PG	-3.86	119.57	132.83
5	A	401	DCP	C2-N3-C4	3.34	119.73	116.34
5	B	401	DCP	O4'-C4'-C5'	2.99	119.22	109.37
5	B	401	DCP	O5'-C5'-C4'	2.96	119.17	108.99
5	A	401	DCP	PB-O3B-PG	-2.93	122.78	132.83
5	A	401	DCP	PB-O3A-PA	-2.55	124.07	132.83
5	B	401	DCP	O3G-PG-O2G	2.15	115.86	107.64
5	B	401	DCP	N4-C4-N3	2.14	119.88	116.49

There are no chirality outliers.

All (7) torsion outliers are listed below:



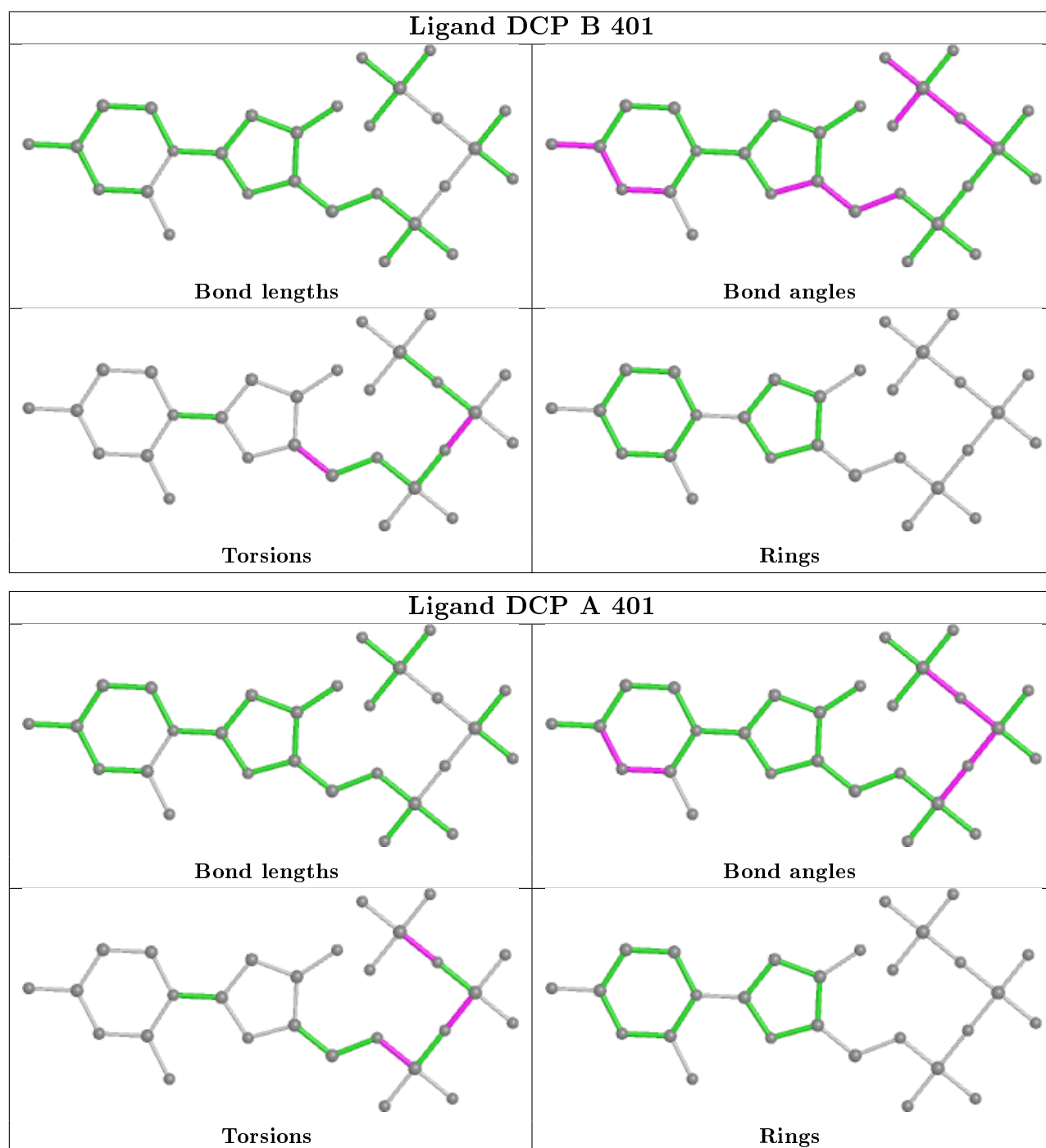
Mol	Chain	Res	Type	Atoms
5	A	401	DCP	PB-O3B-PG-O3G
5	B	401	DCP	C3'-C4'-C5'-O5'
5	B	401	DCP	O4'-C4'-C5'-O5'
5	B	401	DCP	PA-O3A-PB-O1B
5	A	401	DCP	C5'-O5'-PA-O3A
5	B	401	DCP	PA-O3A-PB-O2B
5	A	401	DCP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	401	DCP	4	0
5	A	401	DCP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	16/18 (88%)	0.45	2 (12%) 3 5	47, 66, 135, 137	2 (12%)
1	T	12/18 (66%)	1.80	5 (41%) 0 0	61, 99, 137, 139	4 (33%)
2	D	11/13 (84%)	0.69	2 (18%) 1 1	61, 70, 126, 133	2 (18%)
2	P	10/13 (76%)	3.00	5 (50%) 0 0	50, 99, 123, 127	4 (40%)
3	A	343/348 (98%)	0.31	8 (2%) 60 67	28, 53, 82, 103	3 (0%)
3	B	342/348 (98%)	0.77	43 (12%) 3 5	43, 79, 114, 137	8 (2%)
All	All	734/758 (96%)	0.59	65 (8%) 9 13	28, 64, 112, 139	23 (3%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	213	LEU	7.8
3	B	116	ARG	7.6
2	P	4	DG	7.6
1	T	13	DT	6.4
1	T	16	DC	5.9
3	B	207	SER	5.7
2	P	6	DA	5.4
2	P	3	DG	5.3
2	P	8	DG	5.2
2	D	2	DG	4.0
2	P	5	DG	4.0
3	B	119	ARG	3.8
3	B	212	LYS	3.8
3	B	209	GLU	3.8
3	A	0	HIS	3.8
3	B	295	ILE	3.6
3	B	327	GLU	3.5
3	B	188	ASN	3.5
3	B	296	VAL	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	B	115	VAL	3.4
3	B	278	LYS	3.3
3	B	189	ILE	3.3
1	C	17	DC	3.1
1	T	12	DT	3.1
3	B	292	ASP	3.0
3	B	195	LYS	3.0
1	T	14	DC	2.9
3	B	187	GLY	2.9
3	B	258	LEU	2.8
3	B	241	VAL	2.8
3	A	274	TYR	2.8
3	B	321	LYS	2.7
1	C	16	DC	2.7
2	D	3	DG	2.7
3	B	113	ASP	2.7
1	T	15	DC	2.6
3	B	210	PHE	2.6
3	B	196	LYS	2.6
3	B	192	GLU	2.5
3	B	121	ALA	2.4
3	B	37	PHE	2.4
3	A	318	LEU	2.4
3	B	267	ARG	2.3
3	A	286	VAL	2.3
3	B	215	GLY	2.3
3	B	216	MET	2.3
3	B	206	LEU	2.2
3	A	210	PHE	2.2
3	B	335	VAL	2.2
3	A	253	ARG	2.2
3	B	205	THR	2.2
3	B	117	ASP	2.2
3	B	228	LEU	2.2
3	B	211	ASP	2.2
3	B	208	ILE	2.2
3	B	35	GLY	2.2
3	A	4	LEU	2.1
3	B	325	GLU	2.1
3	B	284	ILE	2.1
3	B	234	ASN	2.1
3	B	230	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	342	GLU	2.1
3	B	324	GLU	2.0
3	B	238	ARG	2.0
3	A	284	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	DOC	D	13	18/19	0.70	0.26	51,57,77,78	3
2	DOC	P	13	18/19	0.76	0.26	85,87,89,91	1
1	EFG	T	5	25/26	0.88	0.14	72,79,100,107	0
1	EFG	C	5	25/26	0.96	0.12	44,50,56,59	0

## 6.3 Carbohydrates [i](#)

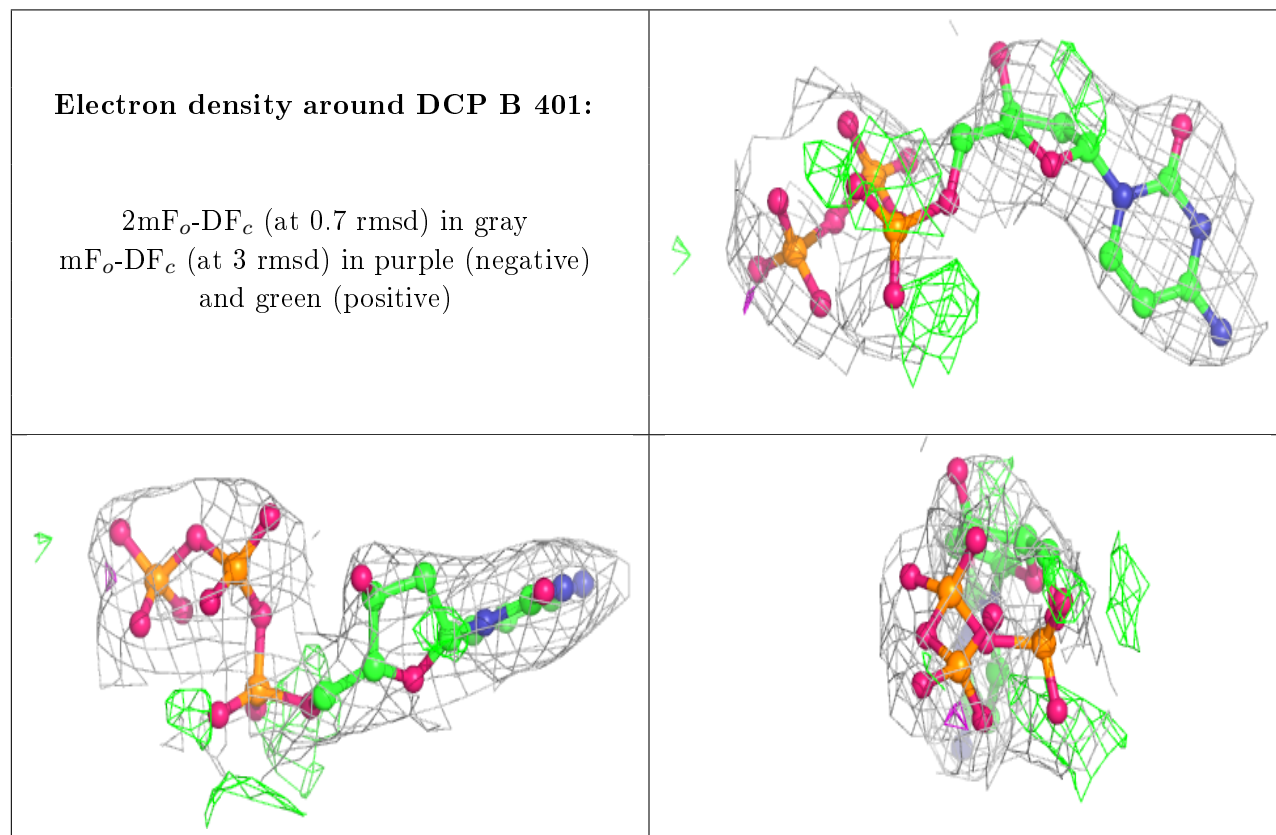
There are no monosaccharides in this entry.

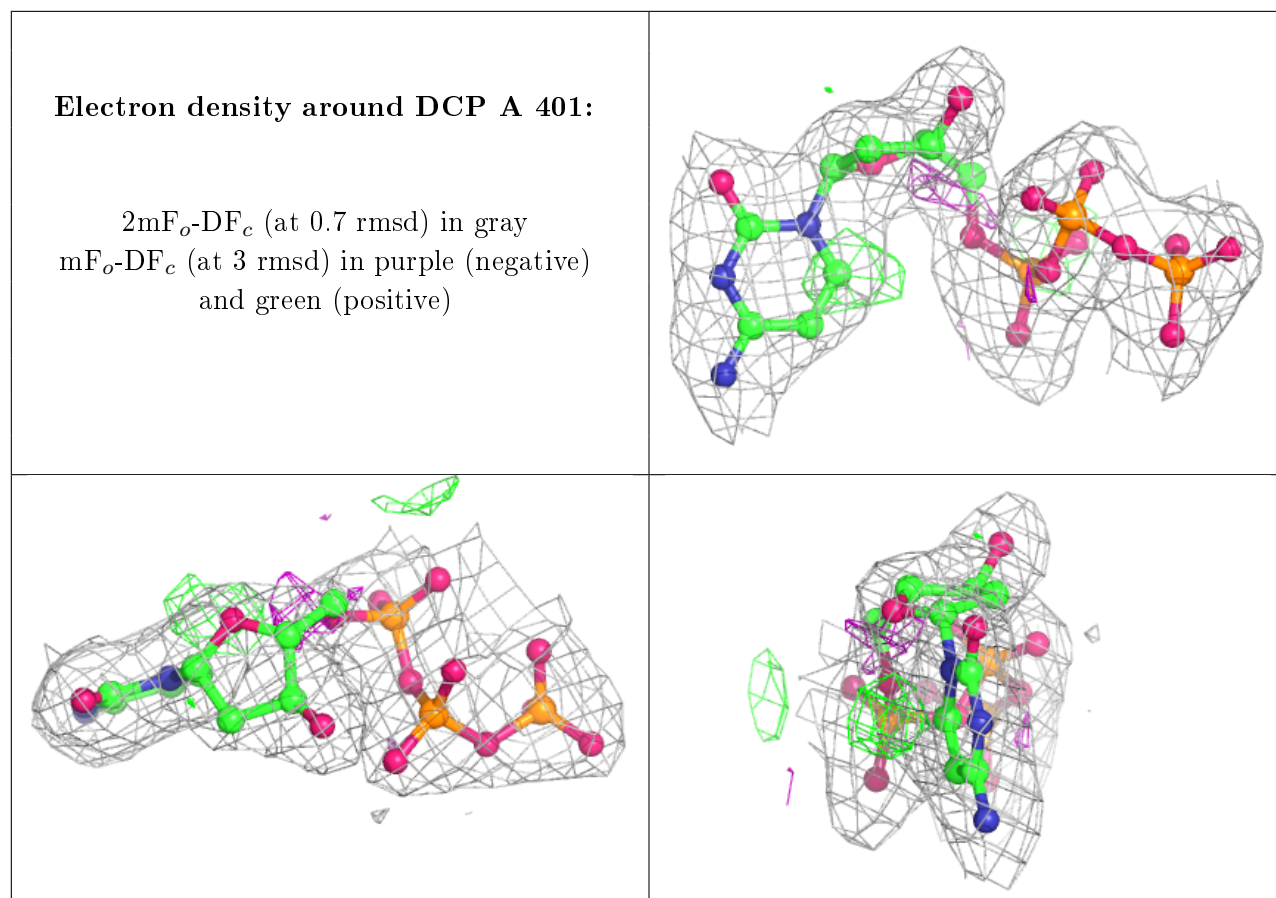
## 6.4 Ligands [i](#)

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
6	MG	B	404	1/1	0.53	0.21	52,52,52,52	0
4	CA	A	404	1/1	0.83	0.15	117,117,117,117	0
4	CA	B	403	1/1	0.84	0.27	77,77,77,77	0
6	MG	A	403	1/1	0.90	0.28	29,29,29,29	0
4	CA	D	101	1/1	0.92	0.22	73,73,73,73	0
5	DCP	B	401	28/28	0.93	0.14	59,67,74,79	0
6	MG	A	402	1/1	0.97	0.17	19,19,19,19	0
5	DCP	A	401	28/28	0.97	0.12	31,46,52,53	0
6	MG	B	402	1/1	0.98	0.23	40,40,40,40	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.





## 6.5 Other polymers ⓘ

There are no such residues in this entry.