



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:19 AM BST

PDB ID : 6UIS  
Title : HIV-1 M184V reverse transcriptase-DNA complex with dCTP  
Authors : Lansdon, E.B.  
Deposited on : 2019-10-01  
Resolution : 2.75 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.

---

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

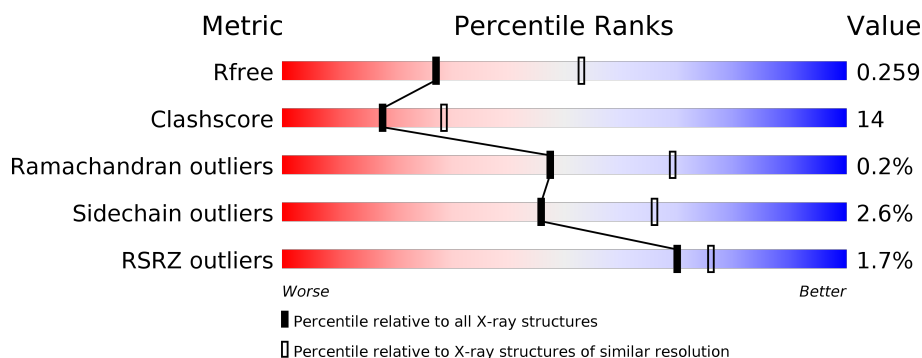
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	572	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 69%, yellow 24%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>1%</span> <span>70%</span> <span>24%</span> <span>• •</span> </div> </div>
2	B	440	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 57%, yellow 29%, orange 1%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>59%</span> <span>29%</span> <span>• 10%</span> </div> </div>
3	P	21	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 62%, yellow 24%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>62%</span> <span>24%</span> <span>14%</span> </div> </div>
4	T	27	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 7%, green 12%, yellow 59%, orange 1%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>7%</span> <span>19%</span> <span>59%</span> <span>• 19%</span> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8733 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 p66 Reverse transcriptase/RNaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4458	2885	743	823	7			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P04585
A	-10	GLY	-	expression tag	UNP P04585
A	-9	SER	-	expression tag	UNP P04585
A	-8	SER	-	expression tag	UNP P04585
A	-7	HIS	-	expression tag	UNP P04585
A	-6	HIS	-	expression tag	UNP P04585
A	-5	HIS	-	expression tag	UNP P04585
A	-4	HIS	-	expression tag	UNP P04585
A	-3	HIS	-	expression tag	UNP P04585
A	-2	HIS	-	expression tag	UNP P04585
A	-1	SER	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585
A	184	VAL	MET	engineered mutation	UNP P04585
A	258	CYS	GLN	engineered mutation	UNP P04585
A	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 2 is a protein called p51 Reverse transcriptase/RNaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	0	0
			3270	2124	546	595	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	184	VAL	MET	engineered mutation	UNP P04585

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P04585

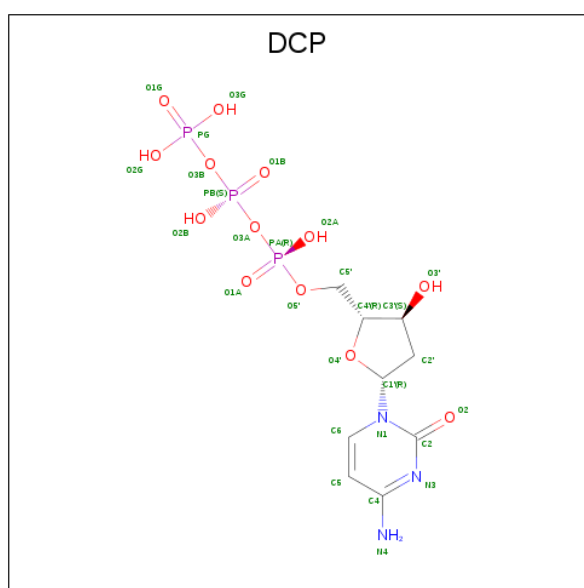
- Molecule 3 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	18	Total	C	N	O	P	0	0	0
			360	172	62	109	17			

- Molecule 4 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	22	Total	C	N	O	P	0	0	0
			460	214	95	129	22			

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula:  $C_9H_{16}N_3O_{13}P_3$ ) (labeled as "Ligand of Interest" by author).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mg	0	0
			2	2		

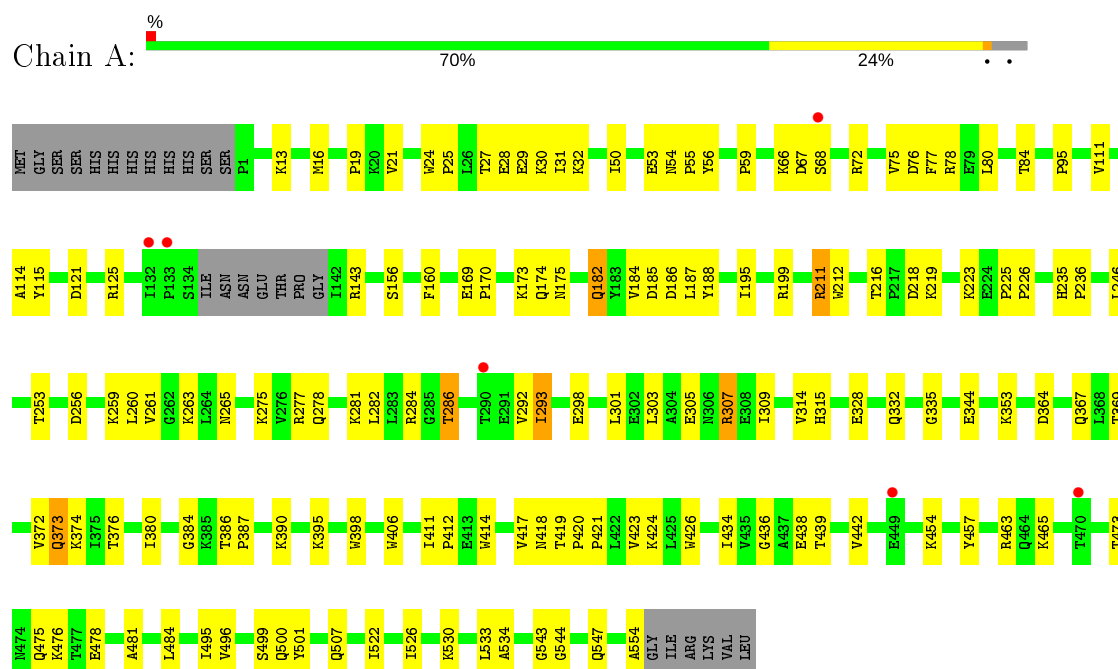
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	86	Total	O	0	0
			86	86		
8	B	41	Total	O	0	0
			41	41		
8	P	8	Total	O	0	0
			8	8		
8	T	10	Total	O	0	0
			10	10		

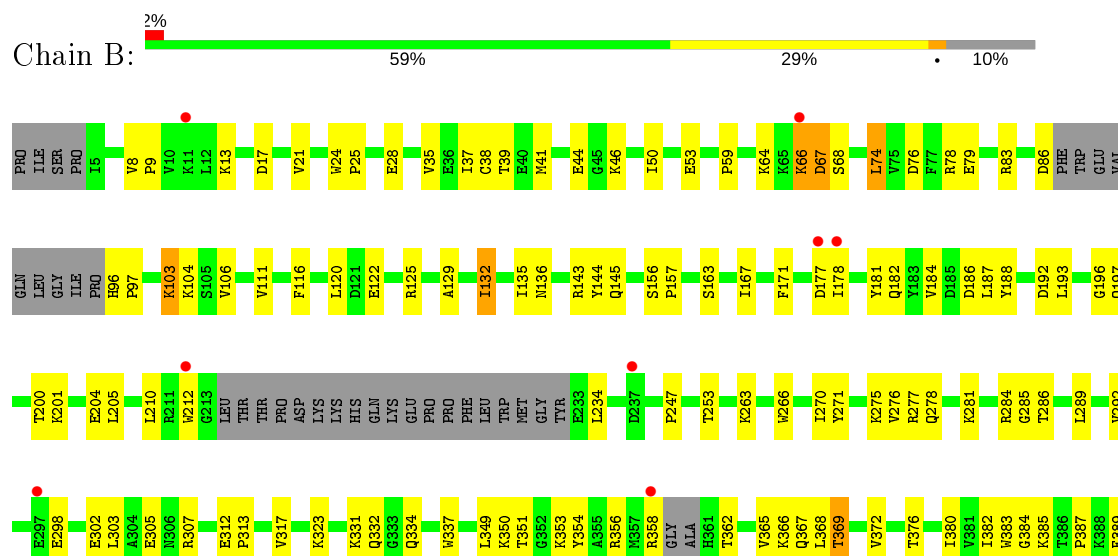
### 3 Residue-property plots

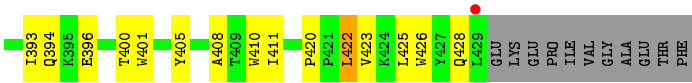
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: p66 Reverse transcriptase/RNaseH

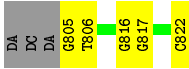


#### • Molecule 2: p51 Reverse transcriptase/RNaseH

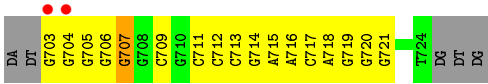




● Molecule 3: Primer DNA



● Molecule 4: Template DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.55Å 169.11Å 103.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.46 – 2.75 47.46 – 2.75	Depositor EDS
% Data completeness (in resolution range)	50.4 (47.46-2.75) 90.8 (47.46-2.75)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692, PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.188 , 0.259 0.190 , 0.259	Depositor DCC
$R_{free}$ test set	2002 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, SO4, DCP

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	0.51	0/4573	0.60	0/6212
2	B	0.46	0/3358	0.57	1/4558 (0.0%)
3	P	0.78	0/381	0.94	0/586
4	T	0.92	1/518 (0.2%)	0.92	1/799 (0.1%)
All	All	0.54	1/8830 (0.0%)	0.64	2/12155 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	709	DC	C3'-O3'	-5.08	1.37	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	67	ASP	N-CA-C	-5.45	96.28	111.00
4	T	707	DG	O4'-C4'-C3'	-5.05	102.48	104.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4458	0	4513	115	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3270	0	3308	100	0
3	P	360	0	203	3	0
4	T	460	0	244	21	0
5	A	28	0	12	1	0
6	A	10	0	0	1	0
7	A	2	0	0	0	0
8	A	86	0	0	2	0
8	B	41	0	0	1	0
8	P	8	0	0	0	0
8	T	10	0	0	0	0
All	All	8733	0	8280	229	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 14.

All (229) 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:A:417:VAL:HG12	1:A:419:THR:HG23	1.48	0.96
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.05	0.91
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.58	0.85
1:A:28:GLU:HA	1:A:31:ILE:HD12	1.58	0.84
1:A:454:LYS:NZ	1:A:554:ALA:HB3	1.96	0.81
2:B:35:VAL:O	2:B:39:THR:HG23	1.80	0.81
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.61	0.81
2:B:354:TYR:OH	2:B:356:ARG:NH1	2.16	0.79
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.64	0.79
1:A:253:THR:HG23	1:A:256:ASP:H	1.48	0.76
1:A:54:ASN:O	1:A:143:ARG:NH2	2.19	0.74
4:T:712:DC:H2'	4:T:713:DC:C6	2.23	0.73
2:B:66:LYS:HE2	2:B:67:ASP:O	1.88	0.72
1:A:478:GLU:HG2	1:A:499:SER:CB	2.20	0.71
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.53	0.71
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.73	0.70
2:B:171:PHE:HE1	2:B:204:GLU:HG2	1.56	0.69
2:B:332:GLN:OE1	2:B:428:GLN:NE2	2.25	0.69
1:A:478:GLU:CG	1:A:499:SER:HB2	2.23	0.68
2:B:278:GLN:HG2	2:B:298:GLU:HB3	1.74	0.68
2:B:66:LYS:HG2	2:B:67:ASP:H	1.58	0.67
2:B:66:LYS:CG	2:B:67:ASP:H	2.07	0.66
2:B:275:LYS:HG3	2:B:302:GLU:HG3	1.77	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:O	1:A:307:ARG:HB2	1.96	0.66
1:A:286:THR:CG2	1:A:293:ILE:HD11	2.25	0.66
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.30	0.66
1:A:260:LEU:HD21	1:A:303:LEU:CD1	2.26	0.65
2:B:275:LYS:HE2	2:B:305:GLU:OE2	1.97	0.65
2:B:365:VAL:O	2:B:369:THR:HG23	1.97	0.65
2:B:167:ILE:HD13	2:B:212:TRP:CD2	2.32	0.64
1:A:286:THR:HG21	1:A:293:ILE:HD11	1.80	0.64
2:B:281:LYS:HG2	2:B:284:ARG:NH1	2.13	0.64
2:B:278:GLN:HG2	2:B:298:GLU:CB	2.28	0.64
1:A:454:LYS:HZ2	1:A:554:ALA:HB3	1.63	0.63
4:T:716:DA:H2'	4:T:717:DC:C6	2.33	0.63
2:B:303:LEU:O	2:B:307:ARG:HG3	1.99	0.62
4:T:711:DC:H2'	4:T:712:DC:C6	2.34	0.62
1:A:76:ASP:OD1	1:A:78:ARG:HG3	1.99	0.62
3:P:805:DG:C2'	3:P:806:DT:H5'	2.30	0.62
3:P:816:DG:H2'	3:P:817:DG:C8	2.34	0.62
1:A:195:ILE:O	1:A:199:ARG:HG3	2.00	0.61
1:A:253:THR:HG22	1:A:256:ASP:OD2	2.01	0.61
2:B:64:LYS:HE2	2:B:68:SER:O	2.00	0.61
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.82	0.60
4:T:716:DA:H2'	4:T:717:DC:H6	1.66	0.60
2:B:24:TRP:HB2	2:B:25:PRO:HD2	1.84	0.60
2:B:66:LYS:HG2	2:B:67:ASP:N	2.17	0.59
1:A:424:LYS:HE3	1:A:426:TRP:CD2	2.37	0.59
1:A:260:LEU:HD21	1:A:303:LEU:HD11	1.84	0.59
1:A:169:GLU:OE2	1:A:173:LYS:HE3	2.04	0.58
1:A:259:LYS:NZ	1:A:263:LYS:HE3	2.18	0.58
1:A:53:GLU:OE1	1:A:53:GLU:N	2.29	0.58
1:A:67:ASP:O	1:A:68:SER:OG	2.21	0.58
4:T:705:DG:C2'	4:T:706:DG:H5'	2.33	0.58
2:B:247:PRO:O	2:B:307:ARG:NH2	2.37	0.58
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.84	0.58
1:A:305:GLU:O	1:A:309:ILE:HG13	2.04	0.58
1:A:438:GLU:OE2	1:A:463:ARG:HD3	2.04	0.58
1:A:500:GLN:HG2	2:B:422:LEU:HD22	1.85	0.57
2:B:323:LYS:O	2:B:385:LYS:NZ	2.37	0.57
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.86	0.57
2:B:163:SER:O	2:B:167:ILE:HG12	2.05	0.57
1:A:417:VAL:HG12	1:A:419:THR:CG2	2.30	0.56
4:T:713:DC:H2'	4:T:714:DG:C8	2.40	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.41	0.56
1:A:406:TRP:HZ3	1:A:507:GLN:HG2	1.71	0.56
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.40	0.56
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.87	0.56
2:B:281:LYS:HE3	2:B:284:ARG:HH12	1.69	0.56
2:B:120:LEU:HD12	2:B:125:ARG:HG2	1.88	0.55
1:A:277:ARG:O	1:A:281:LYS:HG2	2.06	0.55
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.36	0.55
2:B:46:LYS:HE3	2:B:116:PHE:CD2	2.41	0.55
2:B:50:ILE:HD13	2:B:145:GLN:HB3	1.88	0.55
1:A:292:VAL:O	1:A:293:ILE:HG12	2.06	0.55
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.89	0.55
1:A:424:LYS:HE3	1:A:426:TRP:CE2	2.42	0.54
4:T:712:DC:H2'	4:T:713:DC:H6	1.67	0.54
1:A:66:LYS:NZ	8:A:703:HOH:O	2.31	0.54
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.89	0.54
1:A:380:ILE:O	1:A:384:GLY:HA2	2.07	0.54
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.43	0.54
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.43	0.54
1:A:67:ASP:OD1	1:A:68:SER:N	2.40	0.54
1:A:547:GLN:N	1:A:547:GLN:OE1	2.41	0.54
2:B:366:LYS:HD2	2:B:405:TYR:CE1	2.43	0.54
2:B:104:LYS:HG2	2:B:192:ASP:HA	1.90	0.53
2:B:66:LYS:CE	2:B:67:ASP:O	2.56	0.53
1:A:259:LYS:HZ2	1:A:263:LYS:HE3	1.73	0.53
4:T:703:DG:H2'	4:T:703:DG:N3	2.24	0.53
1:A:182:GLN:HG2	1:A:182:GLN:O	2.08	0.53
1:A:186:ASP:O	1:A:187:LEU:HD23	2.08	0.52
2:B:334:GLN:HB3	2:B:358:ARG:HD3	1.91	0.52
2:B:365:VAL:O	2:B:369:THR:CG2	2.58	0.52
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.44	0.52
2:B:380:ILE:O	2:B:384:GLY:HA2	2.09	0.52
1:A:436:GLY:HA2	6:A:602:SO4:O1	2.09	0.52
3:P:805:DG:H2'	3:P:806:DT:H5'	1.91	0.52
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.92	0.51
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.92	0.51
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.92	0.51
1:A:275:LYS:HE2	1:A:332:GLN:NE2	2.26	0.51
1:A:353:LYS:O	1:A:374:LYS:NZ	2.44	0.51
1:A:473:THR:HG23	1:A:476:LYS:HD2	1.92	0.51
1:A:281:LYS:HB3	1:A:284:ARG:HH21	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:LYS:HG2	2:B:351:THR:N	2.26	0.51
1:A:522:ILE:O	1:A:526:ILE:HG13	2.11	0.51
1:A:55:PRO:HG2	1:A:56:TYR:CE2	2.46	0.50
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.45	0.50
1:A:30:LYS:NZ	4:T:704:DG:O6	2.43	0.50
2:B:382:ILE:HG22	2:B:383:TRP:CE2	2.46	0.50
1:A:27:THR:HG22	1:A:29:GLU:H	1.76	0.50
1:A:121:ASP:O	1:A:125:ARG:HG3	2.12	0.50
1:A:253:THR:HG22	1:A:256:ASP:CG	2.32	0.49
1:A:284:ARG:HG3	4:T:714:DG:OP1	2.12	0.49
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.93	0.49
2:B:393:ILE:HG12	2:B:394:GLN:N	2.27	0.49
2:B:66:LYS:CG	2:B:67:ASP:N	2.75	0.49
2:B:181:TYR:O	2:B:188:TYR:N	2.36	0.49
2:B:53:GLU:OE1	2:B:53:GLU:N	2.39	0.49
2:B:156:SER:N	2:B:157:PRO:HD2	2.28	0.49
2:B:362:THR:HG23	2:B:367:GLN:NE2	2.28	0.49
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.43	0.49
2:B:253:THR:HA	2:B:292:VAL:HA	1.95	0.48
2:B:263:LYS:HA	2:B:426:TRP:CZ3	2.48	0.48
2:B:44:GLU:HB2	2:B:46:LYS:HD3	1.94	0.48
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.77	0.48
4:T:715:DA:H2''	4:T:716:DA:C8	2.49	0.48
4:T:713:DC:H2''	4:T:714:DG:H5'	1.96	0.48
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.96	0.48
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.48	0.48
2:B:193:LEU:HB3	2:B:197:GLN:HB3	1.96	0.48
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.96	0.48
1:A:475:GLN:N	1:A:475:GLN:OE1	2.40	0.47
1:A:454:LYS:HZ1	1:A:554:ALA:HB3	1.73	0.47
4:T:711:DC:H2'	4:T:712:DC:H6	1.79	0.47
4:T:720:DG:H2''	4:T:721:DG:H8	1.79	0.47
2:B:266:TRP:CH2	2:B:426:TRP:HB3	2.49	0.47
2:B:201:LYS:O	2:B:204:GLU:HB3	2.15	0.47
2:B:106:VAL:HB	2:B:234:LEU:HB2	1.97	0.47
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.97	0.47
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.49	0.47
2:B:196:GLY:O	2:B:200:THR:OG1	2.25	0.47
2:B:79:GLU:HG3	2:B:83:ARG:NE	2.24	0.47
1:A:420:PRO:CB	1:A:421:PRO:HA	2.45	0.47
1:A:286:THR:HG22	1:A:293:ILE:HD11	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:THR:CG2	1:A:387:PRO:HD2	2.45	0.47
1:A:406:TRP:CZ3	1:A:507:GLN:HG2	2.50	0.47
1:A:465:LYS:HD2	1:A:484:LEU:HD11	1.96	0.47
2:B:167:ILE:HD13	2:B:212:TRP:CE3	2.50	0.47
2:B:376:THR:HB	2:B:410:TRP:CH2	2.51	0.47
2:B:312:GLU:HA	2:B:313:PRO:HD3	1.75	0.46
2:B:420:PRO:C	2:B:422:LEU:H	2.18	0.46
2:B:167:ILE:HG23	2:B:212:TRP:CD1	2.51	0.46
2:B:270:ILE:HG22	2:B:271:TYR:CE1	2.51	0.46
2:B:332:GLN:OE1	2:B:332:GLN:HA	2.15	0.46
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.49	0.46
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.97	0.46
2:B:135:ILE:HB	8:B:514:HOH:O	2.15	0.46
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.97	0.46
1:A:278:GLN:OE1	1:A:281:LYS:HE3	2.15	0.45
2:B:276:VAL:HG23	2:B:276:VAL:O	2.15	0.45
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.46	0.45
1:A:419:THR:O	1:A:419:THR:OG1	2.32	0.45
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.17	0.45
1:A:286:THR:HG21	1:A:293:ILE:CD1	2.46	0.45
1:A:301:LEU:O	1:A:305:GLU:HG3	2.17	0.45
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.53	0.44
1:A:260:LEU:HD11	1:A:303:LEU:HD11	1.98	0.44
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.99	0.44
1:A:314:VAL:HG22	1:A:315:HIS:N	2.33	0.44
2:B:182:GLN:HA	2:B:186:ASP:O	2.18	0.44
4:T:718:DA:H2''	4:T:719:DG:H5''	1.99	0.44
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.99	0.44
2:B:396:GLU:HG2	2:B:396:GLU:H	1.60	0.44
1:A:376:THR:HG23	1:A:386:THR:HG23	2.00	0.44
1:A:29:GLU:O	1:A:32:LYS:HE2	2.17	0.43
1:A:174:GLN:HG2	1:A:175:ASN:ND2	2.33	0.43
4:T:706:DG:H2'	4:T:707:DG:C8	2.54	0.43
1:A:95:PRO:HA	2:B:136:ASN:O	2.19	0.43
4:T:703:DG:H3'	4:T:704:DG:C5'	2.47	0.43
1:A:500:GLN:HG2	2:B:422:LEU:CD2	2.49	0.43
2:B:17:ASP:O	2:B:83:ARG:HD3	2.19	0.43
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.49	0.43
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.83	0.43
2:B:66:LYS:HE2	2:B:67:ASP:H	1.84	0.43
1:A:278:GLN:O	1:A:282:LEU:HD13	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:CA	1:A:31:ILE:HD12	2.41	0.42
2:B:120:LEU:HD12	2:B:125:ARG:CG	2.48	0.42
1:A:211:ARG:HG3	1:A:212:TRP:N	2.33	0.42
1:A:261:VAL:HG12	1:A:265:ASN:ND2	2.33	0.42
2:B:103:LYS:NZ	2:B:177:ASP:O	2.49	0.42
1:A:24:TRP:CZ2	4:T:704:DG:C8	3.08	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.54	0.42
2:B:129:ALA:HA	2:B:144:TYR:O	2.20	0.42
2:B:317:VAL:HG12	2:B:349:LEU:HD23	2.02	0.42
1:A:543:GLY:HA2	1:A:544:GLY:HA2	1.57	0.42
1:A:543:GLY:HA3	2:B:285:GLY:O	2.20	0.41
1:A:218:ASP:HB2	8:A:760:HOH:O	2.18	0.41
1:A:72:ARG:NH2	5:A:601:DCP:O3A	2.53	0.41
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.89	0.41
4:T:720:DG:H2''	4:T:721:DG:C8	2.54	0.41
1:A:13:LYS:HB2	1:A:16:MET:HG3	2.02	0.41
2:B:270:ILE:HG22	2:B:271:TYR:CD1	2.55	0.41
1:A:386:THR:HG23	1:A:387:PRO:HD2	2.03	0.41
1:A:457:TYR:HE2	1:A:484:LEU:HG	1.85	0.41
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.60	0.41
1:A:281:LYS:O	1:A:284:ARG:HB2	2.19	0.41
1:A:495:ILE:HB	1:A:533:LEU:HD23	2.01	0.41
2:B:37:ILE:O	2:B:41:MET:HG3	2.20	0.41
1:A:275:LYS:HE2	1:A:332:GLN:HE21	1.85	0.41
1:A:13:LYS:HE2	1:A:84:THR:O	2.20	0.41
1:A:225:PRO:CB	1:A:226:PRO:HA	2.50	0.41
1:A:278:GLN:HA	1:A:281:LYS:HE3	2.03	0.41
2:B:210:LEU:HD23	2:B:210:LEU:HA	1.89	0.41
2:B:368:LEU:O	2:B:372:VAL:HG23	2.21	0.41
2:B:13:LYS:NZ	2:B:86:ASP:OD1	2.49	0.41
1:A:369:THR:HG22	1:A:373:GLN:OE1	2.21	0.41
2:B:8:VAL:HG12	2:B:9:PRO:O	2.20	0.41
2:B:187:LEU:HA	2:B:187:LEU:HD12	1.90	0.41
4:T:703:DG:C3'	4:T:704:DG:C5'	2.99	0.41
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.56	0.40
2:B:275:LYS:HE3	2:B:302:GLU:HG3	2.03	0.40
2:B:78:ARG:HD3	2:B:411:ILE:O	2.21	0.40
2:B:353:LYS:HG2	2:B:354:TYR:N	2.36	0.40
2:B:74:LEU:HD11	2:B:408:ALA:O	2.22	0.40
4:T:719:DG:H2''	4:T:720:DG:C8	2.56	0.40
2:B:104:LYS:HD2	2:B:192:ASP:C	2.42	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:THR:HG21	2:B:289:LEU:HD13	2.02	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	543/572 (95%)	515 (95%)	27 (5%)	1 (0%)	47	69
2	B	387/440 (88%)	367 (95%)	19 (5%)	1 (0%)	41	61
All	All	930/1012 (92%)	882 (95%)	46 (5%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	VAL
2	B	184	VAL

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/511 (96%)	476 (97%)	13 (3%)	44	65
2	B	361/400 (90%)	352 (98%)	9 (2%)	47	67
All	All	850/911 (93%)	828 (97%)	22 (3%)	46	66



All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	188	TYR
1	A	211	ARG
1	A	216	THR
1	A	219	LYS
1	A	223	LYS
1	A	286	THR
1	A	293	ILE
1	A	298	GLU
1	A	307	ARG
1	A	344	GLU
1	A	373	GLN
1	A	418	ASN
2	B	66	LYS
2	B	74	LEU
2	B	103	LYS
2	B	132	ILE
2	B	277	ARG
2	B	286	THR
2	B	369	THR
2	B	422	LEU
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
3	DOC	P	822	3,4	14,19,20	2.08	6 (42%)	13,26,29	3.61	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
3	DOC	P	822	3,4	-	2/4/18/19	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	822	DOC	C4-N3	4.24	1.42	1.35
3	P	822	DOC	C5-C4	-3.23	1.33	1.41
3	P	822	DOC	O4'-C1'	2.79	1.48	1.42
3	P	822	DOC	O5'-C5'	-2.30	1.39	1.44
3	P	822	DOC	C1'-N1	-2.20	1.42	1.49
3	P	822	DOC	C4-N4	2.09	1.41	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	822	DOC	C2'-C1'-N1	10.15	131.60	112.48
3	P	822	DOC	O4'-C4'-C5'	6.56	120.31	109.52
3	P	822	DOC	C2-N3-C4	2.62	119.00	116.34
3	P	822	DOC	C2'-C3'-C4'	2.08	106.61	102.72

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	822	DOC	O4'-C1'-N1-C6
3	P	822	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z  > 2$
6	SO4	A	603	-	4,4,4	0.17	0	6,6,6	0.15	0
5	DCP	A	601	7	23,29,29	0.85	0	30,45,45	1.36	3 (10%)
6	SO4	A	602	-	4,4,4	0.19	0	6,6,6	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DCP	A	601	7	-	5/19/34/34	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	DCP	C2-N3-C4	3.98	120.38	116.34
5	A	601	DCP	N4-C4-N3	2.41	120.30	116.49
5	A	601	DCP	O3G-PG-O2G	2.20	116.03	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	DCP	PB-O3B-PG-O2G

*Continued on next page...*

*Continued from previous page...*

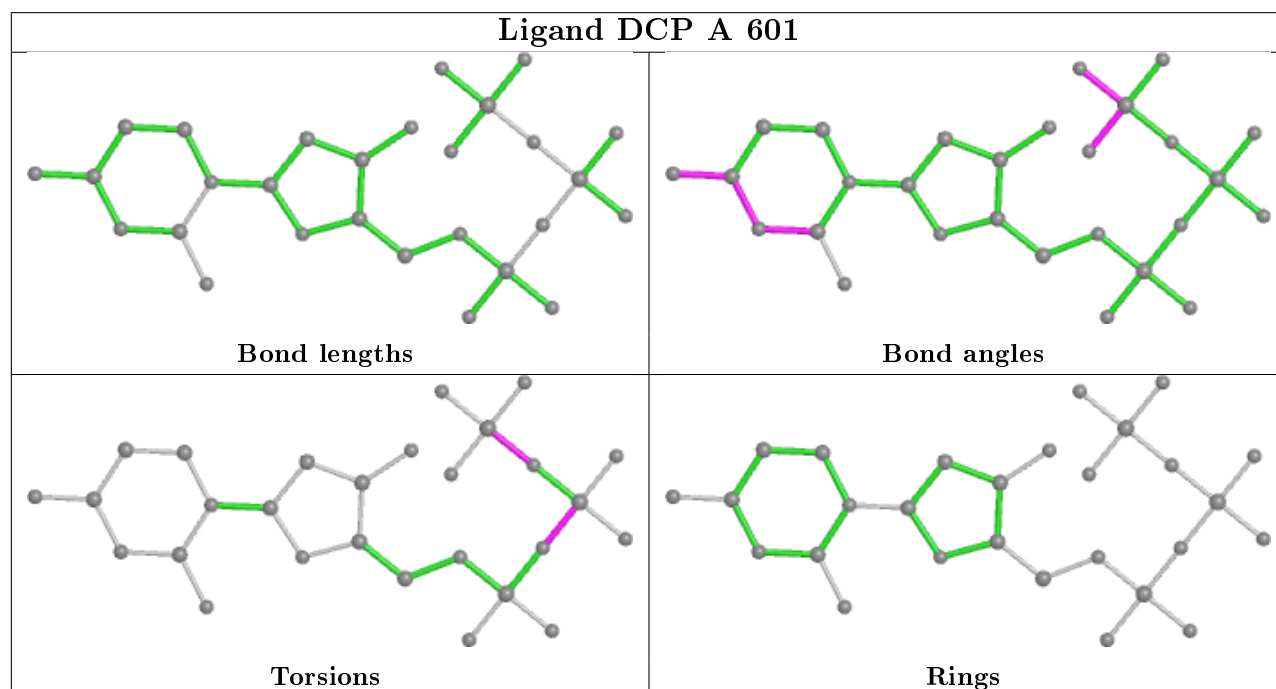
Mol	Chain	Res	Type	Atoms
5	A	601	DCP	PB-O3B-PG-O3G
5	A	601	DCP	PA-O3A-PB-O1B
5	A	601	DCP	PB-O3B-PG-O1G
5	A	601	DCP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	DCP	1	0
6	A	602	SO4	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.



## 5.7 Other polymers

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	547/572 (95%)	-0.25	6 (1%) 80 85	4, 20, 56, 79	0
2	B	395/440 (89%)	-0.03	9 (2%) 60 67	4, 32, 66, 92	0
3	P	17/21 (80%)	-0.74	0 100 100	11, 36, 50, 50	0
4	T	22/27 (81%)	-0.21	2 (9%) 9 9	10, 41, 76, 95	0
All	All	981/1060 (92%)	-0.17	17 (1%) 70 76	4, 25, 62, 95	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	297	GLU	3.9
2	B	66	LYS	3.8
1	A	290	THR	3.6
2	B	358	ARG	3.3
2	B	178	ILE	3.2
2	B	237	ASP	2.8
2	B	177	ASP	2.7
2	B	212	TRP	2.4
4	T	704	DG	2.4
4	T	703	DG	2.3
1	A	68	SER	2.3
2	B	429	LEU	2.3
1	A	449	GLU	2.2
1	A	470	THR	2.2
2	B	11	LYS	2.2
1	A	132	ILE	2.0
1	A	133	PRO	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( $\text{\AA}^2$ )	Q<0.9
3	DOC	P	822	18/19	0.99	0.13	7,11,17,17	0

## 6.3 Carbohydrates [i](#)

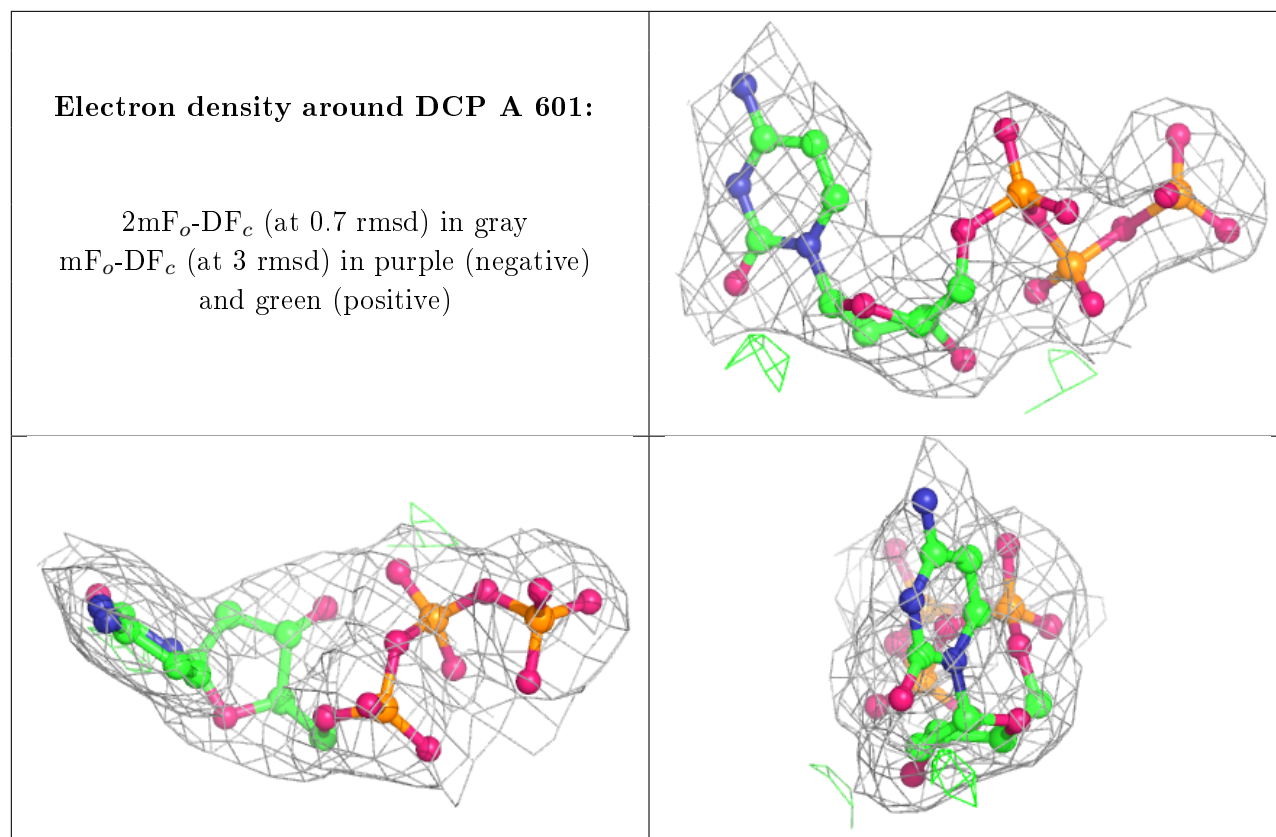
There are no monosaccharides in this entry.

## 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( $\text{\AA}^2$ )	Q<0.9
7	MG	A	605	1/1	0.89	0.14	50,50,50,50	0
6	SO4	A	603	5/5	0.90	0.20	58,59,67,92	0
6	SO4	A	602	5/5	0.97	0.14	23,29,36,48	0
7	MG	A	604	1/1	0.99	0.12	5,5,5,5	0
5	DCP	A	601	28/28	0.99	0.11	8,13,18,26	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 [i](#)

There are no such residues in this entry.