



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:12 am BST

PDB ID : 4PTF  
Title : Ternary crystal structure of yeast DNA polymerase epsilon with template G  
Authors : Jain, R.; Rajashankar, K.R.; Buku, A.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.  
Deposited on : 2014-03-10  
Resolution : 2.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

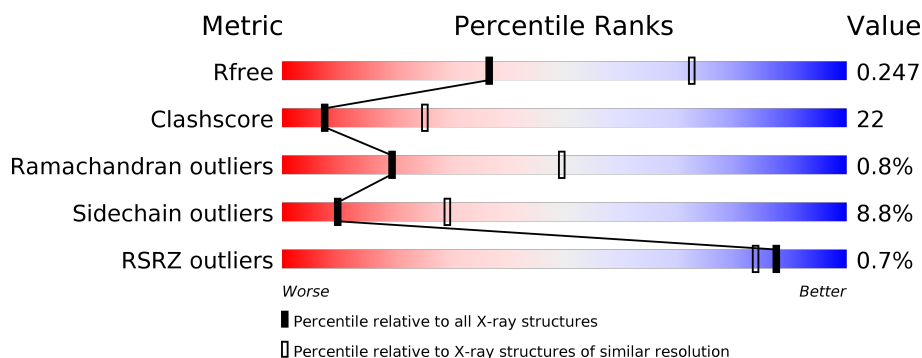
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	1194	<div> <div></div> <div> <div></div> <div>55%</div> <div>34%</div> <div>5%</div> <div>7%</div> </div> </div>
2	P	12	<div> <div>25%</div> <div>58%</div> <div>8%</div> <div>8%</div> </div>
3	T	16	<div> <div>44%</div> <div>50%</div> <div>6%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9572 atoms, of which 6 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 epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1112	Total	C	N	O	S	0	0	0
			8851	5674	1477	1658	42			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P21951
A	-5	PRO	-	EXPRESSION TAG	UNP P21951
A	-4	GLY	-	EXPRESSION TAG	UNP P21951
A	-3	GLY	-	EXPRESSION TAG	UNP P21951
A	-2	ASP	-	EXPRESSION TAG	UNP P21951
A	-1	PRO	-	EXPRESSION TAG	UNP P21951
A	0	HIS	-	EXPRESSION TAG	UNP P21951

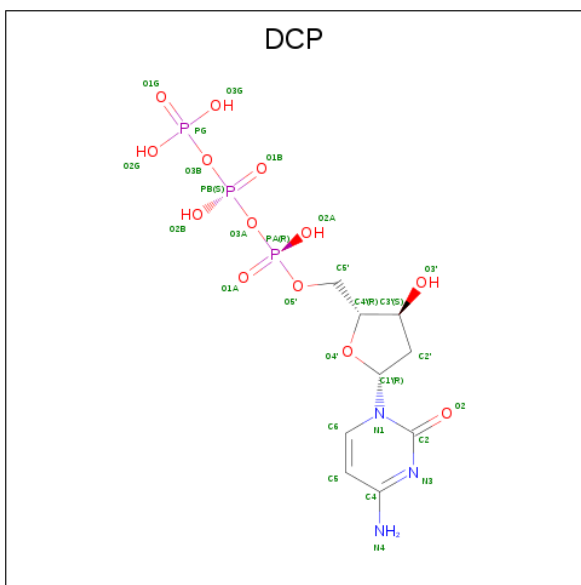
- Molecule 2 is a DNA chain called 5'-D(\*AP\*TP\*CP\*CP\*TP\*CP\*CP\*CP\*CP\*TP\*AP\*(D OC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	P	0	0	0
			213	103	32	67	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	15	Total	C	N	O	P	0	0	0
			318	150	69	85	14			

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Ca	0	0
			3	3		
5	T	1	Total	Ca	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	T	1	Total	C	H	O	0	0
			10	2	6	2		

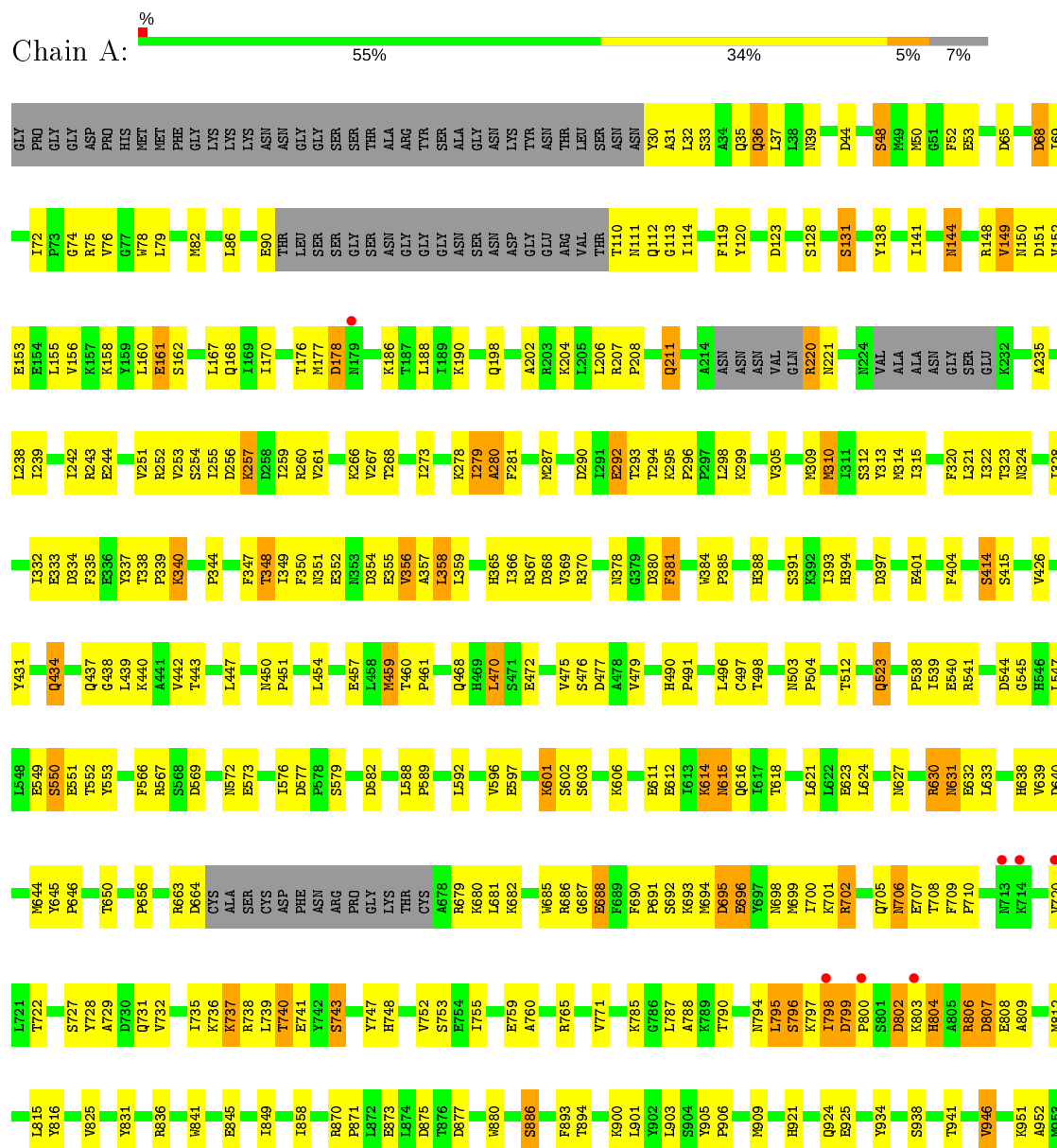
- Molecule 8 is water.

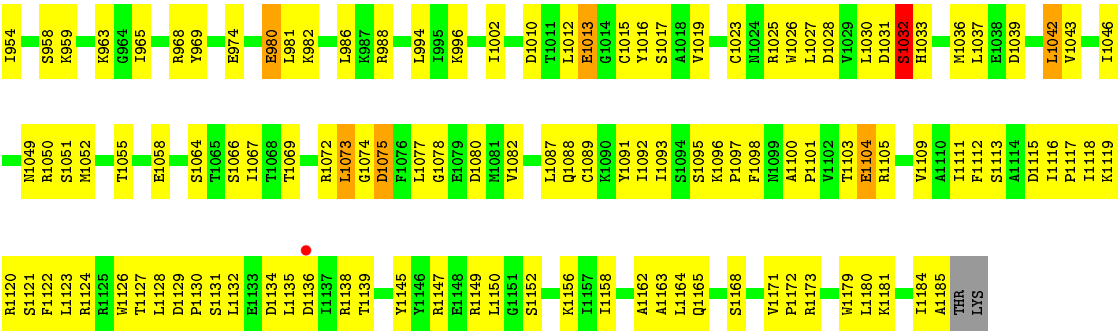
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	121	Total	O	0	0
			121	121		
8	P	8	Total	O	0	0
			8	8		
8	T	18	Total	O	0	0
			18	18		

### 3 Residue-property plots

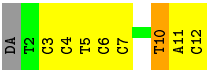
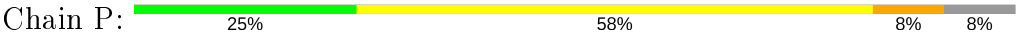
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: DNA polymerase epsilon catalytic subunit A

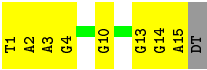




● Molecule 2: 5'-D(\*AP\*TP\*CP\*CP\*TP\*CP\*CP\*CP\*CP\*TP\*AP\*(DOC))-3'



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.29 Å   68.48 Å   149.08 Å 90.00°   109.60°   90.00°	Depositor
Resolution (Å)	46.81 – 2.81 46.81 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.81-2.81) 98.5 (46.81-2.81)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.48 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.183 , 0.247 0.186 , 0.247	Depositor DCC
$R_{free}$ test set	1710 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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, CA, EDO, DCP, NA

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	1/9053 (0.0%)	0.54	0/12265
2	P	1.40	0/215	1.08	1/327 (0.3%)
3	T	1.55	1/360 (0.3%)	0.98	1/557 (0.2%)
All	All	0.61	2/9628 (0.0%)	0.58	2/13149 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	CYS	CB-SG	-5.32	1.73	1.81
3	T	3	DA	C3'-O3'	-5.05	1.37	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	10	DT	O4'-C4'-C3'	-5.33	102.37	104.50
3	T	10	DG	C3'-C2'-C1'	-5.04	96.45	102.50

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	8851	0	8562	397	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	213	0	125	7	0
3	T	318	0	169	4	0
4	A	28	0	12	3	0
5	A	3	0	0	0	0
5	T	1	0	0	0	0
6	A	1	0	0	0	0
7	T	4	6	6	0	0
8	A	121	0	0	15	0
8	P	8	0	0	1	0
8	T	18	0	0	0	0
All	All	9566	6	8874	405	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 22.

All (405) 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:806:ARG:HA	1:A:808:GLU:H	1.08	1.09
1:A:1116:ILE:HG22	1:A:1120:ARG:HD3	1.46	0.98
1:A:806:ARG:HG2	1:A:808:GLU:HB3	1.46	0.98
1:A:980:GLU:HG2	1:A:982:LYS:HE2	1.50	0.93
1:A:611:GLU:O	1:A:615:ASN:ND2	2.04	0.91
1:A:806:ARG:HA	1:A:808:GLU:N	1.85	0.91
1:A:795:LEU:O	1:A:800:PRO:HD3	1.75	0.87
1:A:295:LYS:NZ	1:A:299:LYS:O	2.09	0.86
1:A:576:ILE:HD12	1:A:624:LEU:HD22	1.58	0.84
1:A:576:ILE:CD1	1:A:624:LEU:HD22	2.09	0.82
1:A:1002:ILE:HD11	1:A:1019:VAL:HG13	1.61	0.82
1:A:50:MET:HE3	1:A:370:ARG:HG2	1.59	0.82
1:A:798:ILE:C	1:A:800:PRO:HD2	2.00	0.82
1:A:477:ASP:OD2	8:A:1366:HOH:O	1.98	0.81
1:A:788:ALA:HB2	1:A:816:TYR:HB3	1.62	0.81
1:A:358:LEU:HD23	1:A:359:LEU:N	1.97	0.80
1:A:204:LYS:HG3	1:A:207:ARG:HH12	1.47	0.79
1:A:523:GLN:HG3	8:A:1361:HOH:O	1.81	0.79
1:A:460:THR:HB	1:A:461:PRO:HD3	1.66	0.78
1:A:1116:ILE:HD12	1:A:1116:ILE:H	1.49	0.76
1:A:158:LYS:O	1:A:161:GLU:HB2	1.86	0.76
1:A:708:THR:HG23	1:A:720:VAL:HG13	1.67	0.75
1:A:153:GLU:HG3	1:A:167:LEU:HD21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:LYS:NZ	4:A:1201:DCP:O1G	2.20	0.75
1:A:623:GLU:OE1	1:A:627:ASN:ND2	2.21	0.73
1:A:614:LYS:O	1:A:618:THR:OG1	2.05	0.73
1:A:627:ASN:O	1:A:630:ARG:HD2	1.86	0.73
1:A:1049:ASN:ND2	1:A:1088:GLN:OE1	2.21	0.73
1:A:148:ARG:NE	1:A:151:ASP:OD2	2.20	0.73
1:A:1149:ARG:NH2	8:A:1405:HOH:O	2.20	0.72
1:A:539:ILE:HD11	1:A:729:ALA:HA	1.72	0.72
1:A:202:ALA:O	1:A:206:LEU:HG	1.89	0.72
1:A:708:THR:CG2	1:A:720:VAL:HG13	2.19	0.71
1:A:167:LEU:HD23	1:A:168:GLN:N	2.05	0.71
1:A:693:LYS:H	1:A:696:GLU:HG3	1.54	0.71
1:A:787:LEU:HD12	1:A:788:ALA:N	2.05	0.71
1:A:572:ASN:OD1	8:A:1379:HOH:O	2.09	0.71
1:A:981:LEU:CD2	1:A:986:LEU:HD23	2.20	0.71
1:A:220:ARG:N	1:A:220:ARG:HD3	2.06	0.71
1:A:294:THR:HG22	1:A:309:MET:HE2	1.72	0.71
1:A:790:THR:O	1:A:794:ASN:N	2.20	0.71
1:A:747:TYR:H	1:A:748:HIS:HA	1.56	0.70
1:A:798:ILE:N	1:A:800:PRO:HD2	2.06	0.70
1:A:1097:PRO:HG3	1:A:1128:LEU:HB2	1.73	0.70
1:A:323:THR:OG1	1:A:351:ASN:HA	1.92	0.70
2:P:5:DT:OP2	8:P:108:HOH:O	2.11	0.69
1:A:295:LYS:HE2	1:A:457:GLU:OE2	1.93	0.69
1:A:1138:ARG:HH11	1:A:1138:ARG:HG3	1.58	0.69
1:A:35:GLN:O	1:A:39:ASN:ND2	2.25	0.68
1:A:1025:ARG:NH1	8:A:1344:HOH:O	2.25	0.68
1:A:1116:ILE:HB	1:A:1117:PRO:HD3	1.73	0.68
1:A:1116:ILE:CG2	1:A:1120:ARG:HD3	2.22	0.68
1:A:144:ASN:HD21	1:A:238:LEU:HA	1.59	0.68
1:A:178:ASP:N	1:A:178:ASP:OD1	2.20	0.67
1:A:365:HIS:O	1:A:369:VAL:HG22	1.95	0.67
1:A:545:GLY:HA3	1:A:693:LYS:HE3	1.76	0.67
1:A:332:ILE:HB	1:A:349:ILE:HG21	1.77	0.67
1:A:1103:THR:HG23	3:T:13:DG:OP1	1.94	0.67
1:A:76:VAL:HG23	1:A:266:LYS:HD2	1.77	0.67
1:A:204:LYS:HG3	1:A:207:ARG:NH1	2.09	0.67
1:A:1013:GLU:CD	1:A:1013:GLU:H	1.96	0.66
1:A:728:TYR:O	1:A:732:VAL:HG23	1.95	0.66
1:A:1129:ASP:O	1:A:1132:LEU:HD13	1.96	0.66
1:A:153:GLU:HG3	1:A:167:LEU:CD2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:TYR:CD2	4:A:1201:DCP:H2'2	2.31	0.66
1:A:737:LYS:HA	1:A:740:THR:HG22	1.78	0.66
1:A:802:ASP:HA	1:A:803:LYS:C	2.17	0.66
1:A:257:LYS:HB3	1:A:259:ILE:HD12	1.77	0.65
1:A:475:VAL:O	1:A:479:VAL:HG23	1.97	0.65
1:A:74:GLY:O	1:A:266:LYS:HE3	1.96	0.65
1:A:1100:ALA:O	1:A:1105:ARG:NE	2.26	0.65
1:A:1052:MET:HE2	1:A:1087:LEU:HB3	1.78	0.64
1:A:268:THR:HG21	1:A:273:ILE:HD12	1.80	0.64
1:A:292:GLU:HG3	1:A:459:MET:HE3	1.80	0.63
1:A:806:ARG:CG	1:A:808:GLU:HB3	2.26	0.63
1:A:539:ILE:CD1	1:A:729:ALA:HA	2.27	0.63
1:A:680:LYS:HD3	1:A:759:GLU:OE2	1.99	0.63
1:A:380:ASP:OD2	8:A:1370:HOH:O	2.15	0.63
1:A:696:GLU:OE1	1:A:747:TYR:OH	2.16	0.63
1:A:356:VAL:HG23	1:A:394:HIS:CG	2.34	0.62
1:A:44:ASP:O	1:A:48:SER:OG	2.17	0.62
1:A:737:LYS:HA	1:A:740:THR:CG2	2.29	0.62
1:A:747:TYR:N	1:A:748:HIS:HA	2.15	0.62
1:A:439:LEU:O	1:A:443:THR:OG1	2.08	0.62
1:A:806:ARG:N	1:A:807:ASP:HB2	2.14	0.62
3:T:1:DT:H4'	3:T:2:DA:OP1	1.97	0.62
1:A:1120:ARG:HD2	1:A:1135:LEU:HD21	1.82	0.62
1:A:552:THR:OG1	1:A:553:TYR:N	2.34	0.61
1:A:663:ARG:HA	1:A:664:ASP:CB	2.30	0.61
1:A:539:ILE:HG13	1:A:732:VAL:HG21	1.81	0.61
1:A:334:ASP:OD1	1:A:349:ILE:HG12	2.01	0.61
1:A:332:ILE:N	1:A:351:ASN:OD1	2.34	0.61
1:A:639:VAL:HG12	1:A:946:VAL:HG23	1.81	0.61
1:A:434:GLN:HB2	2:P:10:DT:OP2	2.00	0.61
1:A:739:LEU:HD12	1:A:739:LEU:O	2.01	0.60
1:A:160:LEU:HD11	1:A:206:LEU:HD21	1.82	0.60
1:A:295:LYS:HG2	1:A:296:PRO:O	2.02	0.60
1:A:727:SER:O	1:A:731:GLN:HG3	2.02	0.60
1:A:981:LEU:HD21	1:A:986:LEU:HD23	1.82	0.60
1:A:1036:MET:O	8:A:1335:HOH:O	2.16	0.59
1:A:588:LEU:HB3	1:A:589:PRO:HD3	1.84	0.59
1:A:787:LEU:HD11	1:A:816:TYR:CD1	2.36	0.59
1:A:693:LYS:CG	1:A:694:MET:H	2.14	0.59
1:A:384:TRP:HB2	1:A:385:PRO:HD3	1.83	0.59
1:A:1032:SER:OG	1:A:1036:MET:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:GLY:O	8:A:1412:HOH:O	2.17	0.59
1:A:1097:PRO:HG3	1:A:1128:LEU:CB	2.32	0.59
1:A:702:ARG:HA	1:A:705:GLN:HG3	1.85	0.59
1:A:738:ARG:O	1:A:741:GLU:HG2	2.03	0.59
2:P:6:DC:H2''	2:P:7:DC:H5'	1.84	0.59
1:A:253:VAL:O	1:A:257:LYS:HB2	2.04	0.58
1:A:691:PRO:HD2	1:A:743:SER:OG	2.03	0.58
1:A:812:MET:HA	1:A:812:MET:CE	2.33	0.58
1:A:350:PHE:O	1:A:352:GLU:HG2	2.03	0.58
1:A:577:ASP:OD1	1:A:579:SER:HB3	2.04	0.58
1:A:612:GLU:O	1:A:616:GLN:HG3	2.04	0.57
1:A:1031:ASP:OD2	1:A:1173:ARG:NH2	2.34	0.57
1:A:290:ASP:OD2	8:A:1366:HOH:O	2.18	0.57
1:A:1042:LEU:O	1:A:1042:LEU:HD12	2.03	0.57
1:A:693:LYS:CD	1:A:694:MET:H	2.18	0.57
1:A:700:ILE:HG23	1:A:738:ARG:HG2	1.85	0.57
1:A:701:LYS:NZ	8:A:1363:HOH:O	2.36	0.57
1:A:1023:CYS:SG	1:A:1158:ILE:HD13	2.44	0.57
1:A:706:ASN:HD22	1:A:706:ASN:N	2.01	0.57
1:A:69:ILE:HA	1:A:72:ILE:HD12	1.86	0.56
1:A:367:ARG:NH1	1:A:401:GLU:OE1	2.33	0.56
1:A:257:LYS:HB3	1:A:259:ILE:CD1	2.34	0.56
1:A:268:THR:CG2	1:A:273:ILE:HD12	2.36	0.56
1:A:397:ASP:O	1:A:401:GLU:HG2	2.06	0.56
1:A:597:GLU:HA	1:A:602:SER:O	2.04	0.56
1:A:694:MET:O	1:A:698:ASN:N	2.23	0.56
1:A:693:LYS:HG3	1:A:694:MET:H	1.70	0.56
1:A:36:GLN:HA	1:A:39:ASN:HD22	1.71	0.56
1:A:632:GLU:OE2	1:A:886:SER:OG	2.24	0.56
1:A:235:ALA:HA	1:A:238:LEU:HD12	1.88	0.56
1:A:905:TYR:O	1:A:909:MET:HB3	2.05	0.56
1:A:323:THR:HB	1:A:328:ILE:HG13	1.88	0.56
1:A:1138:ARG:NH1	1:A:1138:ARG:HG3	2.21	0.56
1:A:1072:ARG:HB3	1:A:1126:TRP:CZ2	2.40	0.55
1:A:251:VAL:O	1:A:255:ILE:HG13	2.06	0.55
1:A:1039:ASP:O	1:A:1043:VAL:HG13	2.06	0.55
1:A:160:LEU:O	1:A:162:SER:N	2.40	0.55
1:A:799:ASP:N	1:A:800:PRO:HD2	2.21	0.55
1:A:1075:ASP:OD1	1:A:1075:ASP:N	2.37	0.55
2:P:11:DA:H2''	2:P:12:DOC:O4'	2.06	0.55
1:A:152:VAL:O	1:A:156:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:ARG:HD3	1:A:809:ALA:HB2	1.87	0.54
1:A:736:LYS:O	1:A:740:THR:HG22	2.06	0.54
1:A:799:ASP:N	1:A:800:PRO:CD	2.70	0.54
1:A:279:ILE:O	1:A:280:ALA:HB3	2.07	0.54
1:A:299:LYS:HD2	1:A:1077:LEU:HD22	1.90	0.54
1:A:48:SER:HB3	1:A:53:GLU:OE2	2.06	0.54
1:A:1028:ASP:O	1:A:1032:SER:HB3	2.08	0.54
1:A:994:LEU:HD21	1:A:1030:LEU:HD11	1.90	0.54
1:A:309:MET:HG3	1:A:310:MET:HG2	1.89	0.54
1:A:873:GLU:OE2	8:A:1377:HOH:O	2.18	0.54
1:A:731:GLN:O	1:A:735:ILE:HG13	2.07	0.54
1:A:1123:LEU:O	1:A:1127:THR:OG1	2.18	0.53
1:A:796:SER:O	1:A:800:PRO:HG3	2.09	0.53
1:A:52:PHE:CE2	1:A:128:SER:HB2	2.43	0.53
1:A:426:VAL:HG12	1:A:437:GLN:HG2	1.91	0.53
1:A:1030:LEU:HD12	1:A:1150:LEU:HD23	1.91	0.53
1:A:235:ALA:HA	1:A:238:LEU:CD1	2.39	0.53
1:A:707:GLU:OE2	1:A:738:ARG:NH1	2.40	0.53
1:A:958:SER:HB3	1:A:963:LYS:O	2.08	0.53
1:A:624:LEU:CD2	1:A:630:ARG:HD3	2.39	0.52
1:A:1096:LYS:HA	1:A:1097:PRO:C	2.30	0.52
1:A:1122:PHE:O	1:A:1126:TRP:N	2.37	0.52
1:A:82:MET:HE1	1:A:119:PHE:HE2	1.74	0.52
1:A:144:ASN:ND2	1:A:238:LEU:HA	2.23	0.52
1:A:69:ILE:HD11	1:A:266:LYS:HB2	1.91	0.52
1:A:921:HIS:ND1	1:A:938:SER:OG	2.38	0.52
1:A:355:GLU:HB3	1:A:394:HIS:NE2	2.25	0.52
1:A:1013:GLU:O	1:A:1017:SER:OG	2.25	0.52
1:A:144:ASN:H	1:A:144:ASN:ND2	2.07	0.52
1:A:1072:ARG:HD3	1:A:1126:TRP:CE2	2.45	0.52
1:A:737:LYS:CA	1:A:740:THR:HG22	2.39	0.51
1:A:1116:ILE:CD1	1:A:1116:ILE:H	2.19	0.51
1:A:645:TYR:HB2	1:A:646:PRO:HD3	1.92	0.51
1:A:988:ARG:O	1:A:996:LYS:NZ	2.43	0.51
1:A:1101:PRO:HD2	1:A:1104:GLU:OE1	2.10	0.51
1:A:348:THR:C	1:A:349:ILE:HD13	2.30	0.51
1:A:1184:ILE:O	1:A:1185:ALA:HB2	2.11	0.51
1:A:693:LYS:HG3	1:A:694:MET:N	2.25	0.51
1:A:1013:GLU:N	1:A:1013:GLU:CD	2.63	0.51
1:A:1042:LEU:HD12	1:A:1042:LEU:C	2.29	0.51
1:A:685:TRP:CH2	1:A:687:GLY:HA3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:MET:HE3	1:A:261:VAL:HG23	1.93	0.51
1:A:597:GLU:O	1:A:601:LYS:HA	2.10	0.51
1:A:1116:ILE:N	1:A:1116:ILE:HD12	2.20	0.50
1:A:337:TYR:HD2	1:A:479:VAL:HG21	1.75	0.50
1:A:110:THR:OG1	1:A:111:ASN:N	2.43	0.50
1:A:207:ARG:O	1:A:211:GLN:HG2	2.12	0.50
1:A:1012:LEU:O	1:A:1015:CYS:HB3	2.11	0.50
1:A:693:LYS:CG	1:A:694:MET:N	2.73	0.50
1:A:1030:LEU:HD12	1:A:1150:LEU:CD2	2.41	0.50
1:A:339:PRO:C	1:A:340:LYS:HG2	2.33	0.49
1:A:294:THR:CG2	1:A:309:MET:HE2	2.42	0.49
1:A:951:LYS:HB2	1:A:974:GLU:HA	1.94	0.49
1:A:1031:ASP:C	1:A:1033:HIS:H	2.16	0.49
1:A:787:LEU:HD11	1:A:816:TYR:CE1	2.47	0.49
1:A:393:ILE:HD12	1:A:394:HIS:N	2.28	0.49
1:A:1163:ALA:O	1:A:1165:GLN:N	2.46	0.49
1:A:347:PHE:CZ	1:A:475:VAL:HB	2.47	0.49
1:A:579:SER:O	1:A:582:ASP:HB2	2.12	0.49
1:A:709:PHE:HB3	1:A:710:PRO:HD2	1.95	0.49
1:A:969:TYR:CZ	1:A:982:LYS:HG3	2.48	0.49
1:A:110:THR:HG23	1:A:111:ASN:N	2.28	0.49
1:A:1039:ASP:OD1	1:A:1138:ARG:NH1	2.42	0.48
1:A:148:ARG:O	1:A:151:ASP:HB2	2.13	0.48
1:A:549:GLU:OE1	1:A:550:SER:HB3	2.14	0.48
1:A:695:ASP:O	1:A:699:MET:N	2.31	0.48
1:A:82:MET:CE	1:A:261:VAL:HG23	2.43	0.48
1:A:1037:LEU:O	1:A:1138:ARG:NH2	2.47	0.48
1:A:472:GLU:O	1:A:475:VAL:HG22	2.12	0.48
1:A:968:ARG:HA	1:A:982:LYS:O	2.14	0.48
1:A:1111:ILE:HG23	1:A:1112:PHE:N	2.28	0.48
1:A:310:MET:HE1	1:A:321:LEU:HD11	1.95	0.48
1:A:541:ARG:NE	1:A:551:GLU:OE1	2.43	0.48
1:A:679:ARG:HH11	1:A:679:ARG:HG3	1.79	0.48
1:A:322:ILE:HG22	1:A:358:LEU:HD12	1.95	0.48
1:A:468:GLN:HG3	1:A:468:GLN:O	2.14	0.48
1:A:490:HIS:HB3	1:A:491:PRO:CD	2.43	0.48
1:A:806:ARG:HG2	1:A:808:GLU:CB	2.29	0.48
1:A:1016:TYR:CE1	1:A:1162:ALA:HB2	2.49	0.48
1:A:1116:ILE:O	1:A:1120:ARG:HG2	2.14	0.48
1:A:646:PRO:O	1:A:650:THR:HG23	2.14	0.48
1:A:1046:ILE:O	1:A:1046:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:SER:OG	1:A:259:ILE:O	2.29	0.48
1:A:50:MET:CE	1:A:370:ARG:HA	2.43	0.48
1:A:37:LEU:HG	1:A:86:LEU:HD23	1.96	0.48
1:A:573:GLU:HG2	1:A:631:ASN:OD1	2.14	0.48
1:A:1111:ILE:CG2	1:A:1112:PHE:N	2.77	0.47
1:A:836:ARG:HB2	3:T:4:DG:H4'	1.96	0.47
1:A:294:THR:HG22	1:A:309:MET:CE	2.43	0.47
1:A:207:ARG:CB	1:A:208:PRO:HD3	2.44	0.47
1:A:292:GLU:OE2	1:A:459:MET:HE1	2.14	0.47
1:A:803:LYS:O	1:A:804:HIS:ND1	2.48	0.47
1:A:1132:LEU:N	1:A:1132:LEU:HD12	2.29	0.47
1:A:292:GLU:HG3	1:A:459:MET:CE	2.43	0.47
1:A:1064:SER:OG	1:A:1067:ILE:HG13	2.14	0.47
1:A:1152:SER:O	1:A:1156:LYS:HG3	2.14	0.47
2:P:4:DC:H2''	2:P:5:DT:O5'	2.15	0.47
1:A:75:ARG:NH2	1:A:123:ASP:OD2	2.38	0.47
1:A:176:THR:O	1:A:176:THR:HG22	2.15	0.47
1:A:806:ARG:HD3	1:A:809:ALA:N	2.30	0.47
1:A:1066:SER:OG	8:A:1406:HOH:O	2.20	0.47
1:A:333:GLU:O	1:A:335:PHE:HD1	1.97	0.47
1:A:538:PRO:HG3	1:A:541:ARG:HD2	1.96	0.47
1:A:566:PHE:O	1:A:952:ALA:HA	2.15	0.47
1:A:787:LEU:HD13	1:A:816:TYR:CE2	2.50	0.47
1:A:207:ARG:HB3	1:A:208:PRO:HD3	1.97	0.47
1:A:760:ALA:HB3	1:A:849:ILE:HD11	1.96	0.47
1:A:539:ILE:HG23	1:A:540:GLU:HG2	1.97	0.46
1:A:1120:ARG:O	1:A:1124:ARG:HG3	2.16	0.46
1:A:144:ASN:HD21	1:A:238:LEU:CA	2.27	0.46
1:A:366:ILE:HG22	1:A:367:ARG:N	2.29	0.46
1:A:592:LEU:O	1:A:596:VAL:HG23	2.15	0.46
1:A:954:ILE:N	1:A:954:ILE:HD12	2.31	0.46
1:A:177:MET:CE	1:A:186:LYS:HE2	2.45	0.46
1:A:1181:LYS:O	1:A:1184:ILE:HB	2.16	0.46
1:A:298:LEU:HD23	1:A:298:LEU:N	2.31	0.46
1:A:691:PRO:HB2	1:A:747:TYR:CG	2.50	0.46
1:A:1072:ARG:HD3	1:A:1126:TRP:NE1	2.30	0.46
1:A:112:GLN:OE1	1:A:198:GLN:NE2	2.47	0.46
1:A:393:ILE:HD12	1:A:393:ILE:C	2.36	0.46
1:A:313:TYR:CE2	1:A:320:PHE:HB2	2.51	0.46
1:A:36:GLN:H	1:A:36:GLN:HG2	1.48	0.46
1:A:1016:TYR:CZ	1:A:1162:ALA:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:THR:HG23	1:A:344:PRO:HA	1.97	0.45
1:A:50:MET:HA	1:A:50:MET:HE3	1.98	0.45
1:A:959:LYS:HE3	1:A:1152:SER:HB3	1.98	0.45
1:A:603:SER:H	1:A:606:LYS:CE	2.28	0.45
1:A:645:TYR:CG	4:A:1201:DCP:H2'2	2.51	0.45
1:A:287:MET:HA	1:A:314:MET:O	2.15	0.45
1:A:638:HIS:HB2	1:A:880:TRP:CZ3	2.51	0.45
1:A:1136:ASP:O	1:A:1139:THR:OG1	2.35	0.45
1:A:440:LYS:HG3	1:A:451:PRO:HG2	1.98	0.45
1:A:797:LYS:O	1:A:798:ILE:CB	2.64	0.45
1:A:298:LEU:HD23	1:A:457:GLU:OE1	2.17	0.45
1:A:496:LEU:HA	1:A:496:LEU:HD12	1.67	0.45
1:A:244:GLU:OE1	1:A:252:ARG:NH2	2.50	0.45
1:A:798:ILE:CA	1:A:800:PRO:HD2	2.46	0.45
2:P:3:DC:H2'	2:P:4:DC:C6	2.52	0.45
1:A:1119:LYS:HD2	1:A:1135:LEU:HG	1.97	0.45
1:A:358:LEU:HD23	1:A:359:LEU:H	1.77	0.45
1:A:459:MET:O	1:A:470:LEU:HD13	2.17	0.45
1:A:539:ILE:HG23	1:A:540:GLU:N	2.32	0.45
1:A:177:MET:CE	1:A:186:LYS:HB2	2.47	0.45
1:A:656:PRO:HG2	1:A:841:TRP:HB3	1.99	0.45
2:P:6:DC:H2''	2:P:7:DC:C5'	2.47	0.45
1:A:994:LEU:HD12	1:A:1026:TRP:CZ3	2.52	0.45
1:A:1074:GLY:O	1:A:1078:GLY:N	2.48	0.45
1:A:1134:ASP:O	1:A:1135:LEU:HD12	2.17	0.45
1:A:588:LEU:N	1:A:589:PRO:CD	2.80	0.45
1:A:1072:ARG:HD3	1:A:1126:TRP:CD1	2.52	0.44
1:A:1042:LEU:HD12	1:A:1046:ILE:HG12	1.98	0.44
1:A:588:LEU:HD11	1:A:592:LEU:HD11	1.99	0.44
1:A:612:GLU:HG2	1:A:616:GLN:HE21	1.80	0.44
1:A:1180:LEU:O	1:A:1184:ILE:HG12	2.18	0.44
1:A:252:ARG:HD2	1:A:256:ASP:OD2	2.18	0.44
1:A:279:ILE:HG13	1:A:279:ILE:H	1.53	0.44
1:A:388:HIS:O	1:A:391:SER:HB2	2.18	0.44
1:A:149:VAL:CG1	1:A:150:ASN:N	2.80	0.44
1:A:352:GLU:HB3	1:A:357:ALA:HB3	1.99	0.44
1:A:630:ARG:NH2	1:A:886:SER:OG	2.50	0.44
3:T:14:DG:H2''	3:T:15:DA:C8	2.53	0.44
1:A:708:THR:HG21	1:A:720:VAL:HG13	1.99	0.44
1:A:512:THR:HG21	1:A:825:VAL:HG12	1.99	0.44
1:A:1119:LYS:HE3	1:A:1119:LYS:HB3	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:CG2	1:A:239:ILE:HG23	2.48	0.44
1:A:638:HIS:CE1	1:A:640:ASP:HB2	2.53	0.44
1:A:688:GLU:HA	1:A:752:VAL:O	2.17	0.44
1:A:207:ARG:N	1:A:208:PRO:CD	2.80	0.43
1:A:845:GLU:N	1:A:845:GLU:OE1	2.46	0.43
1:A:925:GLU:O	1:A:934:TYR:HA	2.18	0.43
1:A:79:LEU:HG	1:A:261:VAL:HA	2.00	0.43
1:A:858:ILE:HA	1:A:858:ILE:HD12	1.84	0.43
1:A:893:PHE:HB2	1:A:901:LEU:HB2	2.00	0.43
1:A:1171:VAL:HG12	1:A:1171:VAL:O	2.19	0.43
1:A:155:LEU:HD22	1:A:235:ALA:HB3	2.01	0.43
1:A:795:LEU:O	1:A:797:LYS:N	2.52	0.43
1:A:1082:VAL:HG23	1:A:1082:VAL:O	2.18	0.43
1:A:686:ARG:HG3	1:A:755:ILE:HG13	2.01	0.43
1:A:1098:PHE:O	1:A:1100:ALA:N	2.47	0.43
1:A:30:TYR:O	1:A:31:ALA:HB3	2.19	0.43
1:A:426:VAL:CG1	1:A:437:GLN:HG2	2.49	0.43
1:A:349:ILE:N	1:A:349:ILE:HD13	2.34	0.43
1:A:680:LYS:O	1:A:681:LEU:HD23	2.19	0.43
1:A:806:ARG:HD3	1:A:809:ALA:H	1.84	0.43
1:A:378:ASN:ND2	1:A:381:PHE:CD2	2.87	0.43
1:A:644:MET:SD	1:A:877:ASP:HB3	2.59	0.43
1:A:170:ILE:CD1	1:A:188:LEU:HD12	2.49	0.42
1:A:732:VAL:HG12	1:A:736:LYS:HZ3	1.84	0.42
1:A:211:GLN:H	1:A:211:GLN:HG2	1.58	0.42
1:A:905:TYR:N	1:A:906:PRO:CD	2.83	0.42
1:A:337:TYR:CD2	1:A:479:VAL:HG21	2.54	0.42
1:A:875:ASP:O	1:A:877:ASP:N	2.47	0.42
1:A:490:HIS:HB3	1:A:491:PRO:HD3	2.00	0.42
1:A:567:ARG:HG3	1:A:952:ALA:HB2	2.00	0.42
1:A:893:PHE:O	1:A:900:LYS:HA	2.20	0.42
1:A:1069:THR:O	1:A:1073:LEU:HB2	2.19	0.42
1:A:339:PRO:O	1:A:340:LYS:HG2	2.20	0.42
1:A:138:TYR:CD1	1:A:190:LYS:HE3	2.55	0.42
1:A:252:ARG:HD3	1:A:252:ARG:HA	1.86	0.42
1:A:393:ILE:HD11	1:A:394:HIS:CD2	2.55	0.42
1:A:569:ASP:C	1:A:633:LEU:HD22	2.39	0.42
1:A:1171:VAL:N	1:A:1172:PRO:HD3	2.34	0.42
1:A:170:ILE:HD11	1:A:188:LEU:HD12	2.02	0.42
1:A:765:ARG:HD2	1:A:924:GLN:OE1	2.19	0.42
1:A:1184:ILE:O	1:A:1185:ALA:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ARG:NH1	8:A:1416:HOH:O	2.47	0.42
1:A:78:TRP:CZ2	1:A:281:PHE:HB3	2.54	0.42
1:A:296:PRO:HB2	1:A:299:LYS:HB2	2.02	0.42
1:A:686:ARG:HG3	1:A:755:ILE:CG1	2.49	0.42
1:A:870:ARG:HA	1:A:871:PRO:HD2	1.82	0.42
1:A:1097:PRO:HD3	1:A:1126:TRP:O	2.20	0.41
1:A:701:LYS:O	1:A:705:GLN:HG3	2.19	0.41
1:A:988:ARG:HD2	8:A:1409:HOH:O	2.20	0.41
1:A:1097:PRO:CG	1:A:1128:LEU:HB2	2.45	0.41
1:A:1027:LEU:HD22	1:A:1147:ARG:NE	2.35	0.41
1:A:138:TYR:CG	1:A:190:LYS:HE3	2.54	0.41
1:A:74:GLY:C	1:A:266:LYS:HE3	2.40	0.41
1:A:35:GLN:C	1:A:39:ASN:ND2	2.73	0.41
1:A:690:PHE:HA	1:A:691:PRO:HD3	1.91	0.41
1:A:547:LEU:O	1:A:690:PHE:HD2	2.03	0.41
1:A:1052:MET:HG3	1:A:1089:CYS:SG	2.60	0.41
1:A:1050:ARG:HD3	8:A:1407:HOH:O	2.19	0.41
1:A:404:PHE:CZ	1:A:414:SER:HB3	2.55	0.41
1:A:1055:THR:OG1	1:A:1058:GLU:HG3	2.19	0.41
1:A:1069:THR:HG21	1:A:1091:TYR:HB3	2.03	0.41
1:A:324:ASN:OD1	1:A:354:ASP:HA	2.19	0.41
1:A:438:GLY:O	1:A:442:VAL:HG23	2.21	0.41
1:A:1097:PRO:HG3	1:A:1127:THR:O	2.21	0.41
1:A:1129:ASP:HA	1:A:1130:PRO:HD3	1.72	0.41
1:A:1120:ARG:CD	1:A:1135:LEU:HD21	2.47	0.41
1:A:287:MET:HG3	1:A:315:ILE:CG1	2.51	0.41
1:A:695:ASP:N	1:A:695:ASP:OD1	2.49	0.41
1:A:69:ILE:HA	1:A:72:ILE:CD1	2.49	0.41
1:A:141:ILE:HG12	1:A:242:ILE:HG22	2.02	0.41
1:A:260:ARG:HG3	1:A:498:THR:O	2.21	0.41
1:A:131:SER:OG	1:A:267:VAL:HG11	2.21	0.41
1:A:737:LYS:HE3	1:A:737:LYS:HB2	1.58	0.41
1:A:220:ARG:HB3	1:A:221:ASN:H	1.78	0.41
1:A:959:LYS:O	1:A:1179:TRP:NE1	2.53	0.41
1:A:120:TYR:N	1:A:120:TYR:CD1	2.88	0.41
1:A:440:LYS:HA	1:A:451:PRO:HG3	2.02	0.41
1:A:454:LEU:HD23	1:A:459:MET:HG3	2.03	0.41
1:A:503:ASN:HB2	1:A:504:PRO:HD2	2.02	0.41
1:A:1013:GLU:N	1:A:1013:GLU:OE1	2.55	0.40
1:A:65:ASP:O	1:A:68:ASP:N	2.45	0.40
1:A:787:LEU:HD12	1:A:787:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:THR:O	1:A:447:LEU:HB2	2.22	0.40
1:A:1093:ILE:HG13	1:A:1145:TYR:CE2	2.56	0.40
1:A:293:THR:C	1:A:309:MET:HE3	2.42	0.40
1:A:309:MET:HG3	1:A:310:MET:CG	2.52	0.40
1:A:545:GLY:HA3	1:A:693:LYS:CE	2.48	0.40
1:A:621:LEU:HD23	1:A:621:LEU:HA	1.95	0.40
1:A:592:LEU:HD12	1:A:614:LYS:HG3	2.04	0.40
1:A:86:LEU:HG	1:A:113:GLY:HA3	2.02	0.40
1:A:1012:LEU:O	1:A:1015:CYS:N	2.54	0.40
1:A:1115:ASP:O	1:A:1118:ILE:HB	2.21	0.40
1:A:310:MET:HE2	1:A:310:MET:HB3	1.91	0.40
1:A:68:ASP:O	1:A:72:ILE:HD12	2.21	0.40
1:A:708:THR:CG2	1:A:709:PHE:N	2.84	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	1102/1194 (92%)	1005 (91%)	88 (8%)	9 (1%)	19	49

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	GLU
1	A	798	ILE
1	A	796	SER
1	A	1032	SER
1	A	1109	VAL
1	A	1164	LEU
1	A	795	LEU
1	A	799	ASP

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Mol	Chain	Res	Type
1	A	280	ALA

### 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	943/1069 (88%)	860 (91%)	83 (9%)	10	29

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	33	SER
1	A	36	GLN
1	A	48	SER
1	A	68	ASP
1	A	90	GLU
1	A	114	ILE
1	A	131	SER
1	A	144	ASN
1	A	149	VAL
1	A	178	ASP
1	A	211	GLN
1	A	220	ARG
1	A	257	LYS
1	A	278	LYS
1	A	279	ILE
1	A	292	GLU
1	A	305	VAL
1	A	310	MET
1	A	312	SER
1	A	340	LYS
1	A	348	THR
1	A	356	VAL
1	A	358	LEU
1	A	368	ASP

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Mol	Chain	Res	Type
1	A	381	PHE
1	A	414	SER
1	A	415	SER
1	A	431	TYR
1	A	434	GLN
1	A	450	ASN
1	A	459	MET
1	A	470	LEU
1	A	476	SER
1	A	523	GLN
1	A	544	ASP
1	A	550	SER
1	A	601	LYS
1	A	614	LYS
1	A	615	ASN
1	A	630	ARG
1	A	631	ASN
1	A	682	LYS
1	A	688	GLU
1	A	692	SER
1	A	695	ASP
1	A	696	GLU
1	A	702	ARG
1	A	706	ASN
1	A	722	THR
1	A	737	LYS
1	A	740	THR
1	A	743	SER
1	A	753	SER
1	A	771	VAL
1	A	802	ASP
1	A	804	HIS
1	A	806	ARG
1	A	807	ASP
1	A	815	LEU
1	A	831	TYR
1	A	886	SER
1	A	894	THR
1	A	903	LEU
1	A	941	THR
1	A	946	VAL
1	A	965	ILE

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Mol	Chain	Res	Type
1	A	980	GLU
1	A	1010	ASP
1	A	1013	GLU
1	A	1032	SER
1	A	1042	LEU
1	A	1051	SER
1	A	1073	LEU
1	A	1075	ASP
1	A	1080	ASP
1	A	1092	ILE
1	A	1095	SER
1	A	1104	GLU
1	A	1113	SER
1	A	1121	SER
1	A	1131	SER
1	A	1168	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	144	ASN
1	A	360	GLN
1	A	434	GLN
1	A	706	ASN

### 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
2	DOC	P	12	3,2	14,19,20	2.64	4 (28%)	13,26,29	1.16	2 (15%)

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	12	3,2	-	2/4/18/19	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	12	DOC	O5'-C5'	-5.72	1.30	1.44
2	P	12	DOC	O4'-C4'	-5.19	1.34	1.44
2	P	12	DOC	C4-N3	-4.24	1.28	1.35
2	P	12	DOC	O4'-C1'	-3.75	1.33	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	12	DOC	C5-C4-N3	2.65	124.78	121.72
2	P	12	DOC	C2-N3-C4	2.33	118.70	116.34

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	12	DOC	C3'-C4'-C5'-O5'
2	P	12	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	12	DOC	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 5 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
7	EDO	T	102	-	3,3,3	0.43	0	2,2,2	0.48	0
4	DCP	A	1201	5	23,29,29	1.79	3 (13%)	30,45,45	1.61	5 (16%)

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
7	EDO	T	102	-	-	1/1/1/1	-
4	DCP	A	1201	5	-	4/19/34/34	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1201	DCP	PA-O5'	5.73	1.82	1.59
4	A	1201	DCP	O5'-C5'	-2.99	1.33	1.44
4	A	1201	DCP	C4-N4	2.21	1.41	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1201	DCP	C2-N3-C4	4.26	120.66	116.34
4	A	1201	DCP	O5'-PA-O1A	-3.83	94.10	109.07
4	A	1201	DCP	C2'-C3'-C4'	-3.35	95.78	102.76
4	A	1201	DCP	C2'-C1'-N1	-2.41	108.72	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1201	DCP	O2A-PA-O5'	-2.18	97.60	107.75

There are no chirality outliers.

All (5) torsion outliers are listed below:

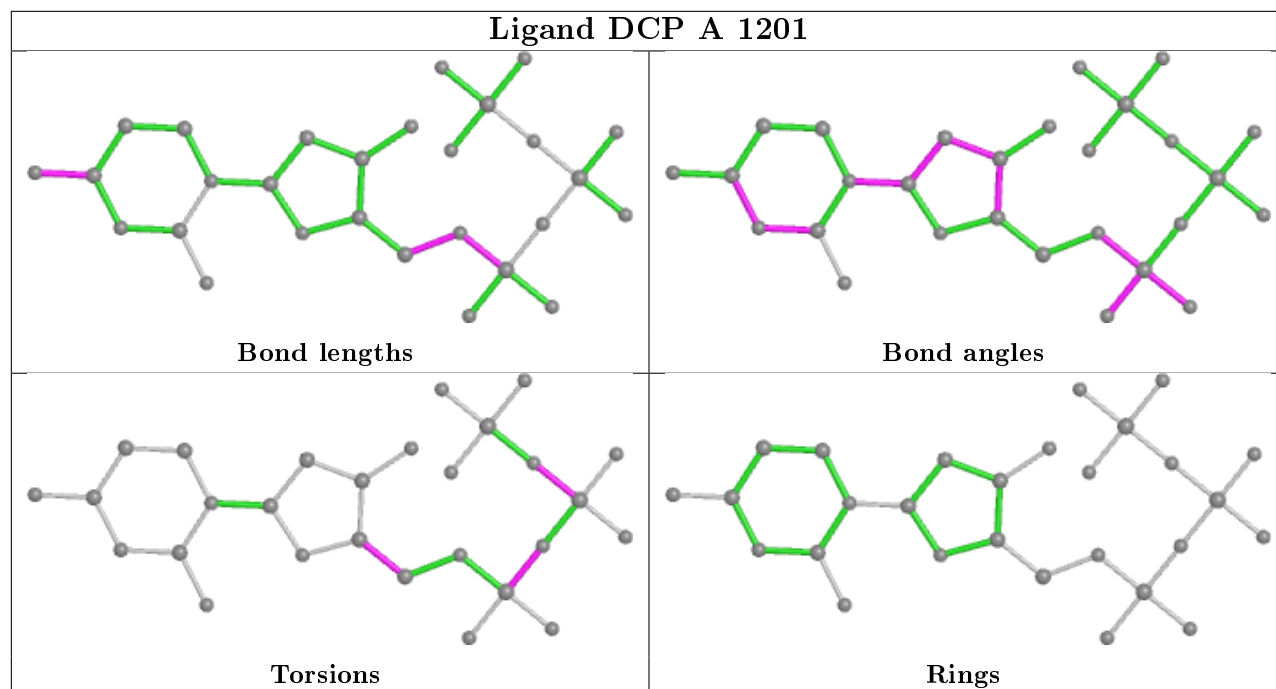
Mol	Chain	Res	Type	Atoms
4	A	1201	DCP	O4'-C4'-C5'-O5'
4	A	1201	DCP	PG-O3B-PB-O1B
4	A	1201	DCP	PG-O3B-PB-O2B
7	T	102	EDO	O1-C1-C2-O2
4	A	1201	DCP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1201	DCP	3	0

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



## 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	1112/1194 (93%)	-0.31	8 (0%) 87 84	22, 47, 78, 126	0
2	P	10/12 (83%)	-0.51	0 100 100	25, 37, 79, 90	0
3	T	15/16 (93%)	-0.31	0 100 100	22, 33, 61, 64	0
All	All	1137/1222 (93%)	-0.31	8 (0%) 87 84	22, 46, 78, 126	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	800	PRO	4.2
1	A	803	LYS	3.8
1	A	714	LYS	3.2
1	A	713	ASN	2.6
1	A	720	VAL	2.5
1	A	798	ILE	2.5
1	A	1136	ASP	2.4
1	A	179	ASN	2.1

### 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	P	12	18/19	0.98	0.21	19,25,31,40	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

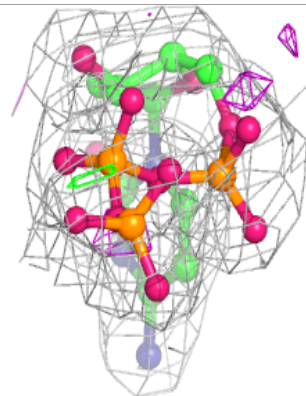
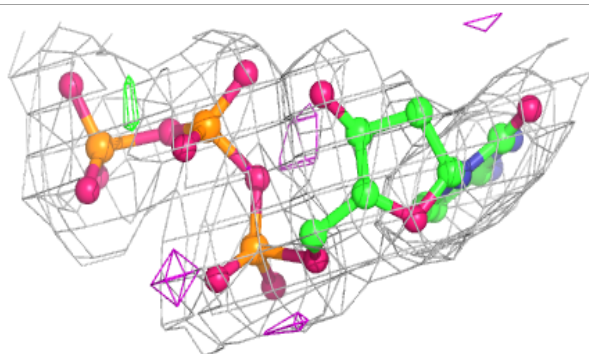
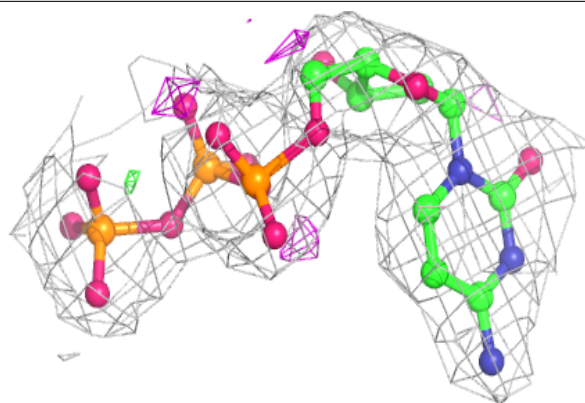
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	T	102	4/4	0.86	0.17	59,70,73,73	0
5	CA	A	1203	1/1	0.92	0.08	68,68,68,68	0
5	CA	A	1202	1/1	0.93	0.11	49,49,49,49	0
6	NA	A	1205	1/1	0.95	0.16	26,26,26,26	0
5	CA	A	1204	1/1	0.95	0.19	64,64,64,64	0
5	CA	T	101	1/1	0.97	0.08	67,67,67,67	0
4	DCP	A	1201	28/28	0.98	0.19	20,26,37,41	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 DCP A 1201:**

$2mF_o-DF_c$  (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.