

Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 09:13 AM EDT

PDB ID	:	4RNO
Title	:	Crystal structure of human polymerase eta extending an abasic site-dA pair
		by inserting dCTP opposite template G
Authors	:	Patra, A.; Egli, M.
Deposited on	:	2014-10-24
Resolution	:	2.82 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

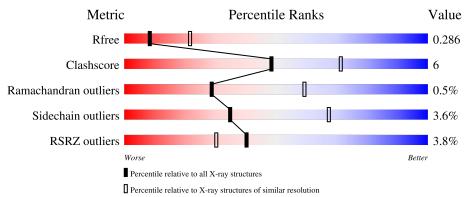
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: : : : :	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.82 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3617 (2.84 - 2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	А	435	80%	16% ••
2	Т	12	58% 33%	8%
3	Р	8	88%	12%



4RNO

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3801 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called DNA polymerase eta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	425	Total 3329	C 2087	N 598	O 621	S 23	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9Y253
А	-1	PRO	-	expression tag	UNP Q9Y253
А	0	HIS	-	expression tag	UNP $Q9Y253$

• Molecule 2 is a DNA chain called Nucleic acids Template: CATG(3DR)TGACGCT.

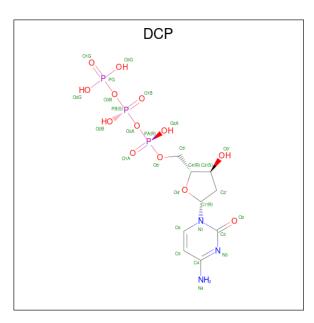
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Т	12	Total 218	C 103	N 37	O 67	Р 11	0	0	1

• Molecule 3 is a DNA chain called Nucleic acids Primar: AGCGTCAA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	Р	8	Total 162	C 78	N 33	0 44	Р 7	0	0	0

• Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



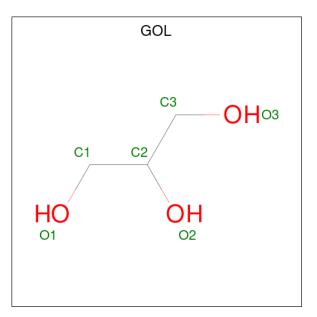


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	Δ	1	Total	С	Ν	Ο	Р	0	0
4	A	1	28	9	3	13	3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Ca 1 1	0	0

• Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	А	1	Total 6	$\begin{array}{c} \mathrm{C} \\ \mathrm{3} \end{array}$	O 3	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	49	Total O 49 49	0	0
7	Т	6	Total O 7 7	0	1
7	Р	1	Total O 1 1	0	0

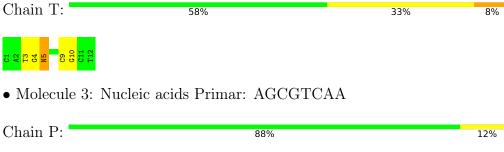


3 Residue-property plots (i)

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.

С	h٤	i	n	A	.:	4	%	_																8	30'	%																				1	.6%	6			• •	•				
GLY	PRO HTS	M		Q5	D6	R7		M14		F17		E22	Q23	R24		P27		R30	-	148		R61	<u>S62</u>		D67		K70		n74	4	079	r r	N OC	487		D120	L121	T122		L132	GLN	6134	C 1 1	72.17	P154	THR	THR	ALA	GLU	GLU	T160		E164	M166	R167	K168
-	L183 T184	S185	P186	-	V197	E198		1204		T208		1216		K224	L225	A226		L229	-	0235		H240	G241	S242	4140	F247		M250		1.25.8		F290	1.230	K293	N294		A300	-	1305	E306		P309	1215	P316		C321	<mark>5322</mark>	K323	N324		L331	A332	T333	1004 1	D355	
N359	LAGG	V367	V368	S369	I370	R371		D375	K376	R377	L378	S379	8380		C385		K394	-	D398	A399	F400		K404	N405	C406	N407	T408		T411	0412 0412	T413	F414		S416	PRO	P418	L419	T420	M421	L422	F423	TA OT	1421 1421	OZ EVI	S432											
•	Ν	[0	le	ec	ul	le	2	2:	ľ	Ň١	10	el	ei	с	8	ıc	i	ds	3	Т	'ei	m	p	lŧ	at	e		С	:A	\]	[(3	;)	3I)]	R)]	[(3.	A	С	G	С	T	I											

• Molecule 1: DNA polymerase eta





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
$\begin{array}{c} \text{Cell constants} \\ \text{a, b, c, } \alpha, \beta, \gamma \end{array}$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness (in resolution range)	89.8 (42.78-2.82) 88.8 (42.78-2.82)	Depositor EDS
R _{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) > 1$	1.03 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1810)	Depositor
R, R_{free}	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor DCC
R_{free} test set	477 reflections (4.88%)	wwPDB-VP
Wilson B-factor $(Å^2)$	69.6	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 25.0	EDS
L-test for twinning ²	$< L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.069 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3801	wwPDB-VP
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: 3DR, DCP, GOL, CA

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				
	Unann	RMSZ	# Z > 5	RMSZ	# Z > 5			
1	А	0.21	0/3384	0.41	0/4563			
2	Т	0.52	0/230	0.90	0/352			
3	Р	0.54	0/182	0.83	0/279			
All	All	0.27	0/3796	0.49	0/5194			

There are no bond length outliers.

There are no bond angle outliers.

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	А	3329	0	3372	41	0
2	Т	218	0	122	5	0
3	Р	162	0	91	1	0
4	А	28	0	12	0	0
5	А	1	0	0	0	0
6	А	6	0	8	0	0
7	А	49	0	0	0	0
7	Р	1	0	0	0	0
7	Т	7	0	0	0	0
All	All	3801	0	3605	44	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 6.

All (44) 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)
2:T:5:3DR:C4'	2:T:5:3DR:O4'	1.67	1.20
1:A:67:ASP:HA	1:A:70:LYS:HE2	1.72	0.71
1:A:366:LEU:HB3	1:A:385:CYS:HB3	1.82	0.61
1:A:166:MET:O	1:A:168:LYS:N	2.34	0.60
1:A:394:LYS:NZ	1:A:398:ASP:OD2	2.37	0.58
1:A:120:ASP:OD1	1:A:122:THR:OG1	2.24	0.56
1:A:371:ARG:HG2	1:A:420:THR:HB	1.86	0.56
2:T:4:DG:H1'	2:T:5:3DR:H1'2	1.89	0.54
1:A:427:THR:OG1	1:A:428:LYS:N	2.39	0.54
1:A:197:VAL:HG21	1:A:216:ILE:HG12	1.88	0.53
1:A:62:SER:HB2	2:T:3:DT:H72	1.91	0.53
1:A:24:ARG:O	1:A:30:ARG:NH2	2.43	0.52
1:A:375:ASP:OD2	1:A:380:SER:OG	2.23	0.51
1:A:86:LYS:NZ	1:A:87:ALA:O	2.41	0.50
1:A:204:ILE:O	1:A:208:THR:OG1	2.25	0.49
1:A:142:LEU:HD23	1:A:198:GLU:HG3	1.95	0.49
1:A:324:ASN:N	2:T:5:3DR:OP2	2.39	0.48
1:A:5:GLN:HB3	1:A:186:PRO:HB3	1.97	0.47
1:A:300:ALA:HB1	1:A:305:ILE:HB	1.98	0.46
1:A:27:PRO:HA	1:A:30:ARG:NE	2.29	0.46
1:A:419:LEU:HD13	1:A:422:LEU:HD21	1.97	0.46
1:A:400:PHE:O	1:A:404:LYS:N	2.48	0.46
1:A:293:LYS:HE2	1:A:293:LYS:HB2	1.85	0.46
1:A:86:LYS:HB3	1:A:323:LYS:HD3	1.97	0.45
1:A:164:GLU:OE2	1:A:167:ARG:NE	2.49	0.45
1:A:224:LYS:NZ	3:P:8:DA:OP1	2.34	0.45
1:A:6:ASP:OD2	1:A:6:ASP:N	2.50	0.45
2:T:9:DC:H2"	2:T:10:DG:C8	2.51	0.45
1:A:333:THR:HA	1:A:414:GLU:HA	1.99	0.45
1:A:7:ARG:NH1	1:A:306:GLU:O	2.49	0.45
1:A:355:ASP:OD1	1:A:359:ASN:ND2	2.49	0.44
1:A:185:SER:HA	1:A:186:PRO:HD3	1.87	0.44
1:A:366:LEU:O	1:A:385:CYS:N	2.50	0.44
1:A:7:ARG:NH2	1:A:309:PRO:HA	2.33	0.44
1:A:226:ALA:HA	1:A:229:LEU:HD12	2.01	0.43
1:A:294:ASN:N	1:A:294:ASN:OD1	2.52	0.43
1:A:48:ILE:O	1:A:61:ARG:HD3	2.20	0.42

Continued on next page...



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:MET:HB2	1:A:17:PHE:HB2	2.02	0.41
1:A:247:PHE:HA	1:A:250:MET:HB3	2.02	0.41
1:A:198:GLU:HG2	1:A:235:GLN:NE2	2.36	0.41
1:A:322:SER:HB3	1:A:423:PHE:HD2	1.85	0.41
1:A:293:LYS:H	1:A:293:LYS:HG3	1.64	0.40
1:A:315:LEU:HA	1:A:316:PRO:HD3	1.89	0.40
1:A:290:PHE:HB2	1:A:294:ASN:HB2	2.03	0.40

Continued from previous page...

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	А	419/435~(96%)	386~(92%)	31 (7%)	2~(0%)	29 59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	166	MET
1	А	167	ARG

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	А	364/372~(98%)	351~(96%)	13~(4%)	35 67			

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	6	ASP
1	А	74	ASP
1	А	79	GLN
1	А	122	THR
1	А	240	HIS
1	А	242	SER
1	А	294	ASN
1	А	306	GLU
1	А	321	CYS
1	А	334	ARG
1	А	378	LEU
1	А	411	ILE
1	А	413	THR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	В	Bond lengths Bond angles								
10101	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2				
2	3DR	Т	5	2	8,11,12	5.87	5 (62%)	9,14,17	1.18	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
2	3DR	Т	5	2	-	0/3/15/16	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Т	5	3DR	O4'-C4'	13.83	1.67	1.44
2	Т	5	3DR	C3'-C4'	-7.00	1.33	1.53
2	Т	5	3DR	O4'-C1'	-3.87	1.31	1.42
2	Т	5	3DR	C2'-C1'	3.27	1.60	1.51
2	Т	5	3DR	C2'-C3'	2.53	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Т	5	3DR	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is 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	Iol Type Chain Res Linl			Link	Bond lengths			Bond angles		
IVIOI	Mol Type Chain K	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
4	DCP	А	501	5	25,29,29	3.41	12 (48%)	37,45,45	1.11	4 (10%)
6	GOL	А	503	-	$5,\!5,\!5$	0.38	0	5,5,5	0.34	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
4	DCP	А	501	5	-	7/22/34/34	0/2/2/2
6	GOL	А	503	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
4	А	501	DCP	O4'-C1'	7.94	1.60	1.42
4	А	501	DCP	C2'-C1'	-7.50	1.31	1.52
4	А	501	DCP	C3'-C4'	-6.13	1.36	1.53
4	А	501	DCP	C6-C5	4.95	1.46	1.35
4	А	501	DCP	C2-N3	4.74	1.46	1.36
4	А	501	DCP	C4-N3	4.30	1.43	1.34
4	А	501	DCP	C4-N4	4.18	1.43	1.33
4	А	501	DCP	O4'-C4'	3.46	1.52	1.45
4	А	501	DCP	C2-N1	3.07	1.46	1.40
4	А	501	DCP	C2'-C3'	3.06	1.61	1.52
4	А	501	DCP	C1'-N1	-3.05	1.40	1.48
4	А	501	DCP	C6-N1	2.09	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	А	501	DCP	PB-O3B-PG	-2.47	124.34	132.83
4	А	501	DCP	C2'-C3'-C4'	2.41	107.79	102.76
4	А	501	DCP	PB-O3A-PA	-2.41	124.56	132.83
4	А	501	DCP	C3'-C2'-C1'	2.23	108.13	102.54

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms					
4	А	501	DCP	C5'-O5'-PA-O1A					
	Continued on next page								

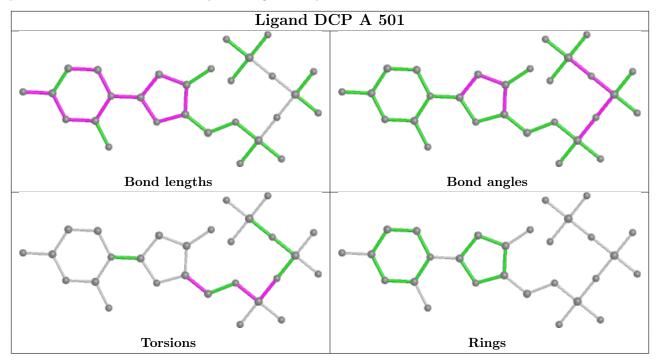
Mol	Chain	Res	Type	Atoms
4	А	501	DCP	C5'-O5'-PA-O2A
6	А	503	GOL	O1-C1-C2-C3
4	А	501	DCP	O4'-C4'-C5'-O5'
4	А	501	DCP	C3'-C4'-C5'-O5'
4	А	501	DCP	PB-O3A-PA-O1A
6	А	503	GOL	O1-C1-C2-O2
4	А	501	DCP	PB-O3A-PA-O5'
4	А	501	DCP	C5'-O5'-PA-O3A

Continued from previous page...

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	425/435~(97%)	0.34	17 (4%) 38 28	45, 55, 79, 96	0
2	Т	$11/12 \ (91\%)$	-0.03	0 100 100	52, 55, 101, 104	0
3	Р	8/8 (100%)	-0.45	0 100 100	50, 53, 59, 59	0
All	All	444/455~(97%)	0.32	17 (3%) 40 30	45, 55, 80, 104	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	416	SER	4.4
1	А	408	THR	4.1
1	А	369	SER	3.9
1	А	415	TRP	3.5
1	А	419	LEU	3.5
1	А	370	ILE	3.3
1	А	368	VAL	3.0
1	А	331	LEU	2.9
1	А	407	ASN	2.9
1	А	406	CYS	2.7
1	А	378	LEU	2.7
1	А	377	ARG	2.7
1	А	380	SER	2.5
1	А	379	SER	2.2
1	А	183	LEU	2.1
1	А	258	LEU	2.1
1	А	22	GLU	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^{th} 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	$B-factors(Å^2)$	Q < 0.9
2	3DR	Т	5	11/12	0.94	0.16	59,61,62,63	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

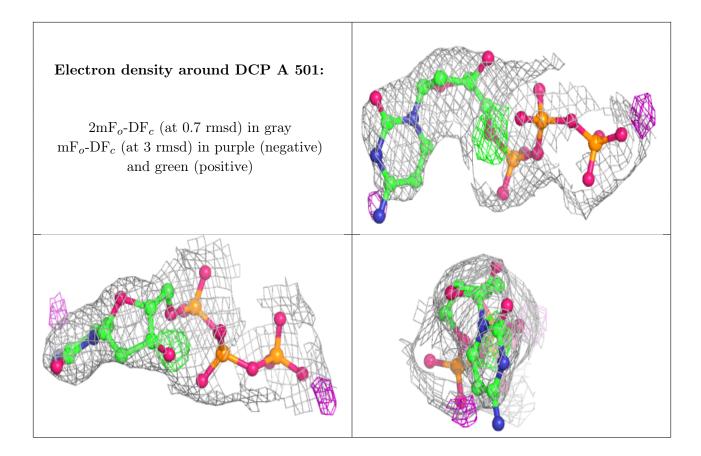
6.4 Ligands (i)

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^{th} 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	$B-factors(Å^2)$	Q < 0.9
6	GOL	А	503	6/6	0.70	0.15	$58,\!64,\!67,\!68$	0
5	CA	А	502	1/1	0.93	0.12	47,47,47,47	0
4	DCP	А	501	28/28	0.94	0.20	47,49,57,59	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.

