



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:05 am BST

PDB ID : 3OJU  
Title : Snapshot of the large fragment of DNA polymerase I from *Thermus Aquaticus* processing c5 modified thymidies  
Authors : Marx, A.; Diederichs, K.; Obeid, S.  
Deposited on : 2010-08-23  
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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

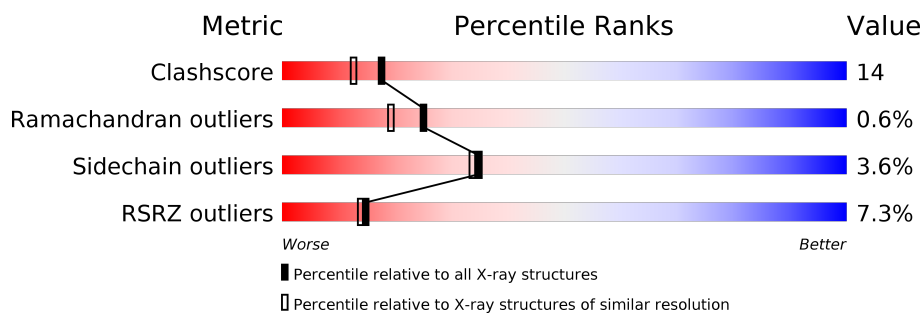
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	540	<div> <div>7%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
2	B	12	<div> <div>67%</div> <div>33%</div> </div>
3	C	16	<div> <div>6%</div> <div>44%</div> <div>44%</div> <div>13%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9574 atoms, of which 4435 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 I, thermostable.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	539	Total	C	H	N	O	S	0	0	0
			8612	2723	4326	771	779	13			

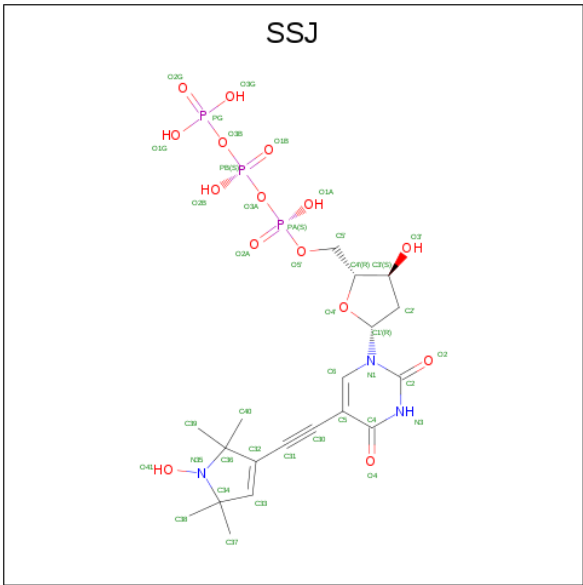
- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*AP\*CP\*CP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*(DOC))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	12	Total	C	H	N	O	P	0	0	0
			252	114	12	48	67	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	P	0	0	0
			290	136	56	84	14			

- Molecule 4 is 2'-deoxy-5-[(1-hydroxy-2,2,5,5-tetramethyl-2,5-dihydro-1H-pyrrol-3-yl)ethynyl]uridine 5'-(tetrahydrogen triphosphate) (three-letter code: SSJ) (formula: C<sub>19</sub>H<sub>28</sub>N<sub>3</sub>O<sub>15</sub>P<sub>3</sub>).

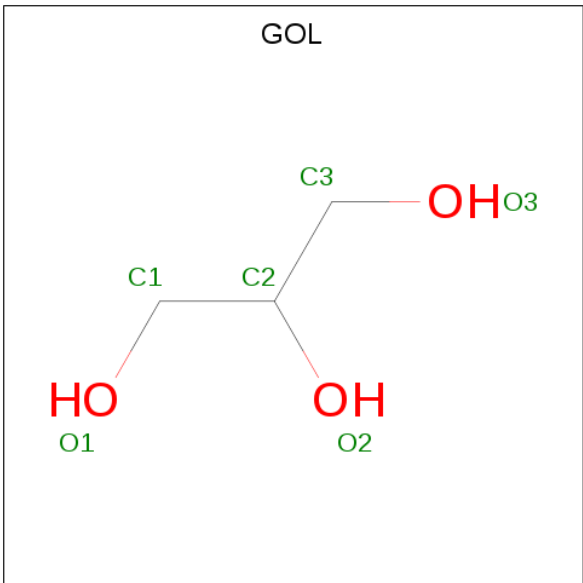


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			40	19	3	15	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

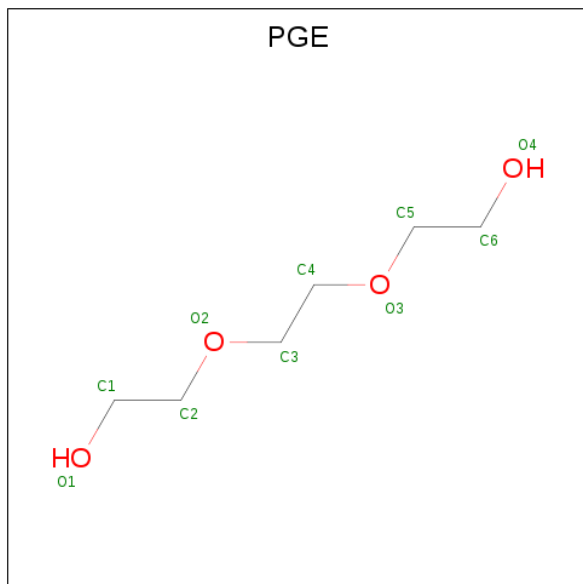
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			8	2	4	2		
7	A	1	Total	C	H	O	0	0
			8	2	4	2		
7	A	1	Total	C	H	O	0	0
			8	2	4	2		
7	A	1	Total	C	H	O	0	0
			8	2	4	2		
7	A	1	Total	C	H	O	0	0
			10	4	4	2		
7	A	1	Total	C	H	O	0	0
			8	2	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			8	2	4	2		
7	A	1	Total	C	H	O	0	0
			8	2	4	2		
7	A	1	Total	C	H	O	0	0
			8	2	4	2		
7	A	1	Total	C	H	O	0	0
			8	2	4	2		
7	C	1	Total	C	H	O	0	0
			17	5	9	3		

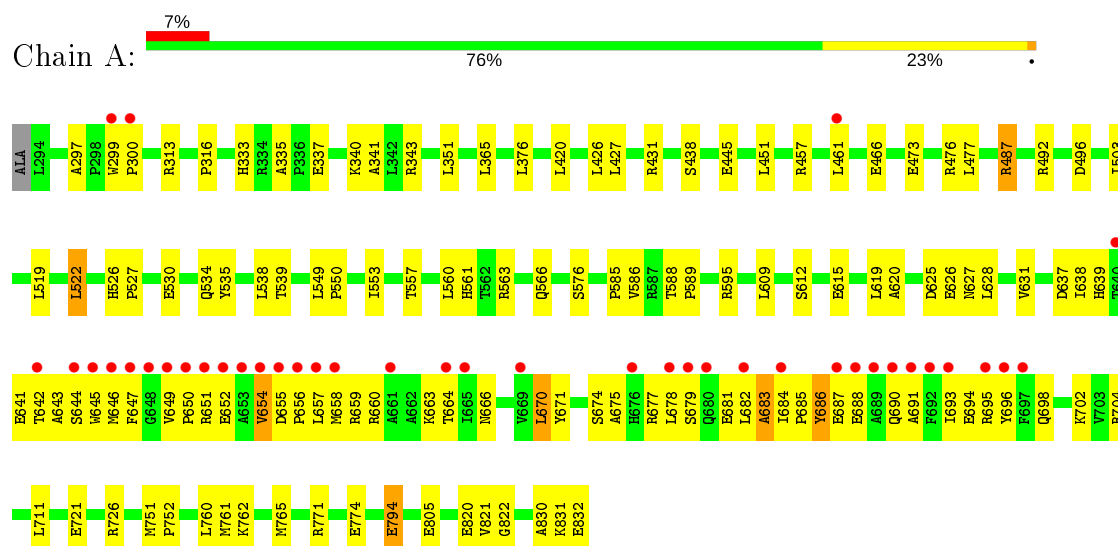
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	158	Total	O	0	0
			158	158		
8	B	15	Total	O	0	0
			15	15		
8	C	22	Total	O	0	0
			22	22		

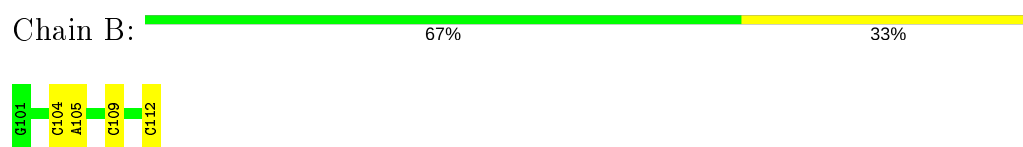
### 3 Residue-property plots [i](#)

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.

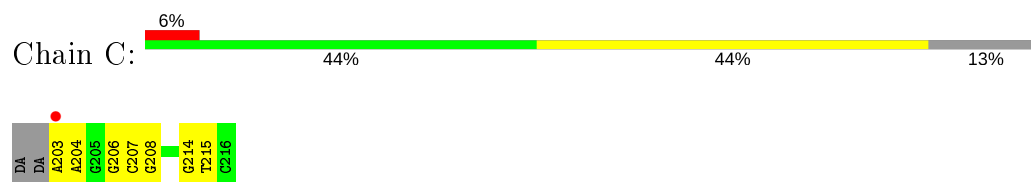
- Molecule 1: DNA polymerase I, thermostable



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.02Å 109.02Å 91.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.21 – 2.00 47.21 – 2.00	Depositor EDS
% Data completeness (in resolution range)	75.1 (47.21-2.00) 75.1 (47.21-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.177 , 0.219 0.177 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: GOL, MG, PGE, SSJ, DOC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/4376	0.49	0/5927
2	B	0.49	0/249	1.12	1/382 (0.3%)
3	C	0.55	0/325	1.07	0/500
All	All	0.29	0/4950	0.60	1/6809 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	DC	O4'-C1'-N1	5.54	111.88	108.00

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	4286	4326	4336	119	0
2	B	240	12	134	3	0
3	C	290	0	157	11	0
4	A	40	0	24	10	0
5	A	2	0	0	0	0
6	A	30	40	40	2	0
6	C	6	8	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	42	40	40	1	0
7	C	8	9	9	4	0
8	A	158	0	0	7	0
8	B	15	0	0	1	0
8	C	22	0	0	0	0
All	All	5139	4435	4748	133	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 (133) 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)
3:C:203:DA:H2''	3:C:204:DA:OP1	1.47	1.11
1:A:343:ARG:NH1	1:A:365:LEU:HD11	2.04	0.73
1:A:762:LYS:HA	1:A:765:MET:HE3	1.72	0.71
3:C:206:DG:C8	7:C:2:PGE:H5	2.26	0.70
1:A:557:THR:OG1	1:A:561:HIS:HE1	1.77	0.68
3:C:203:DA:H2'	3:C:203:DA:N3	2.08	0.67
1:A:609:LEU:HD12	1:A:821:VAL:HB	1.77	0.67
1:A:626:GLU:OE2	1:A:702:LYS:HE3	1.94	0.67
1:A:687:GLU:O	1:A:691:ALA:HB3	1.95	0.66
1:A:686:TYR:O	1:A:687:GLU:HB3	1.99	0.62
1:A:644:SER:HA	1:A:649:VAL:CG2	2.30	0.62
1:A:335:ALA:HB1	1:A:341:ALA:HB2	1.81	0.62
1:A:316:PRO:HD2	1:A:563:ARG:HD3	1.82	0.62
1:A:644:SER:HA	1:A:649:VAL:HG22	1.82	0.61
1:A:694:GLU:O	1:A:698:GLN:HG3	2.01	0.61
1:A:678:LEU:HD21	1:A:693:ILE:HG13	1.84	0.60
1:A:337:GLU:HG3	1:A:340:LYS:NZ	2.17	0.60
1:A:466:GLU:HG2	1:A:538:LEU:HD21	1.84	0.59
1:A:473:GLU:O	1:A:477:LEU:HD13	2.01	0.59
1:A:609:LEU:CD1	1:A:821:VAL:HB	2.33	0.59
1:A:685:PRO:CB	1:A:686:TYR:HA	2.33	0.59
6:C:1:GOL:H11	7:C:2:PGE:H6	1.85	0.59
1:A:761:MET:HG3	1:A:765:MET:HE2	1.86	0.58
1:A:794:GLU:CD	1:A:794:GLU:H	2.07	0.58
1:A:625:ASP:HB2	1:A:702:LYS:HB2	1.85	0.57
1:A:762:LYS:HA	1:A:765:MET:CE	2.33	0.57
1:A:376:LEU:HD22	1:A:420:LEU:HD22	1.87	0.56
1:A:627:ASN:O	1:A:631:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HD11	1:A:522:LEU:HD13	1.86	0.56
1:A:647:PHE:CZ	1:A:658:MET:HA	2.41	0.56
1:A:619:LEU:HD22	1:A:670:LEU:HD11	1.87	0.55
1:A:678:LEU:CD1	1:A:693:ILE:HD11	2.37	0.55
1:A:822:GLY:HA3	1:A:830:ALA:O	2.07	0.55
3:C:207:DC:OP2	7:C:2:PGE:H6	2.07	0.54
1:A:615:GLU:CD	4:A:1:SSJ:H2'A	2.29	0.54
1:A:694:GLU:HA	1:A:694:GLU:OE1	2.07	0.53
3:C:214:DG:C8	3:C:215:DT:H72	2.43	0.53
1:A:671:TYR:O	3:C:204:DA:H2''	2.08	0.53
3:C:203:DA:C2'	3:C:204:DA:OP1	2.35	0.53
1:A:666:ASN:O	1:A:670:LEU:HB2	2.08	0.53
1:A:642:THR:O	1:A:646:MET:HG3	2.08	0.52
1:A:503:ILE:CD1	1:A:522:LEU:HD13	2.40	0.52
1:A:476:ARG:NH2	1:A:477:LEU:HD11	2.25	0.52
1:A:576:SER:O	3:C:208:DG:H4'	2.10	0.51
1:A:831:LYS:O	1:A:832:GLU:HB2	2.10	0.51
1:A:686:TYR:C	1:A:688:GLU:H	2.14	0.51
1:A:659:ARG:HD3	8:A:53:HOH:O	2.10	0.51
1:A:664:THR:CG2	4:A:1:SSJ:H40B	2.41	0.50
1:A:677:ARG:O	1:A:681:GLU:HG2	2.11	0.50
1:A:503:ILE:HD11	1:A:522:LEU:CD1	2.41	0.50
1:A:620:ALA:HA	1:A:628:LEU:HD23	1.94	0.50
1:A:343:ARG:HH11	1:A:365:LEU:HD11	1.72	0.50
1:A:670:LEU:HD13	1:A:671:TYR:CZ	2.47	0.50
4:A:1:SSJ:H38B	2:B:112:DOC:OP2	2.12	0.50
1:A:639:HIS:CD2	8:A:120:HOH:O	2.64	0.50
1:A:691:ALA:O	1:A:695:ARG:HG3	2.12	0.49
1:A:299:TRP:CZ2	1:A:341:ALA:HB1	2.47	0.49
1:A:427:LEU:HD21	1:A:431:ARG:NH2	2.28	0.49
1:A:585:PRO:O	1:A:595:ARG:HD3	2.11	0.49
1:A:664:THR:HG21	4:A:1:SSJ:C40	2.43	0.49
1:A:337:GLU:HG3	1:A:340:LYS:CE	2.43	0.48
1:A:685:PRO:HA	1:A:688:GLU:HB2	1.94	0.48
1:A:678:LEU:HD13	1:A:693:ILE:HD11	1.94	0.48
1:A:638:ILE:HB	8:A:120:HOH:O	2.14	0.48
3:C:206:DG:OP2	7:C:2:PGE:H42	2.13	0.48
1:A:645:TRP:CZ2	1:A:695:ARG:HD3	2.49	0.47
1:A:337:GLU:HG3	1:A:340:LYS:HE2	1.97	0.47
1:A:655:ASP:OD1	1:A:656:PRO:HD2	2.15	0.47
1:A:420:LEU:HD11	1:A:426:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:SER:HB2	1:A:685:PRO:CG	2.45	0.47
1:A:445:GLU:O	1:A:561:HIS:HD2	1.98	0.47
1:A:626:GLU:CD	1:A:626:GLU:H	2.18	0.47
1:A:751:MET:HB3	1:A:752:PRO:HD3	1.97	0.47
1:A:625:ASP:HA	1:A:702:LYS:HG3	1.97	0.47
1:A:451:LEU:HB3	1:A:553:ILE:HD11	1.96	0.47
1:A:466:GLU:HG2	1:A:538:LEU:CD2	2.45	0.46
2:B:104:DC:H2''	2:B:105:DA:C8	2.50	0.46
1:A:563:ARG:HD2	8:A:32:HOH:O	2.15	0.46
1:A:457:ARG:O	1:A:461:LEU:HD13	2.15	0.46
1:A:625:ASP:CB	1:A:702:LYS:HB2	2.45	0.46
1:A:297:ALA:HB3	1:A:333:HIS:CD2	2.51	0.46
1:A:721:GLU:HA	1:A:726:ARG:O	2.15	0.46
1:A:637:ASP:O	1:A:641:GLU:HG3	2.16	0.45
1:A:492:ARG:O	1:A:496:ASP:HB2	2.16	0.45
1:A:337:GLU:HG3	1:A:340:LYS:HZ1	1.80	0.45
4:A:1:SSJ:H5'A	2:B:112:DOC:C2'	2.45	0.45
1:A:588:THR:HB	1:A:589:PRO:HD2	1.99	0.45
1:A:655:ASP:HB3	1:A:658:MET:HG3	1.99	0.45
1:A:761:MET:O	1:A:765:MET:HG3	2.16	0.45
1:A:691:ALA:HA	1:A:694:GLU:HB3	1.98	0.44
6:A:6:GOL:H2	8:B:27:HOH:O	2.17	0.44
1:A:675:ALA:O	1:A:678:LEU:HB2	2.17	0.44
1:A:654:VAL:HA	1:A:658:MET:SD	2.57	0.44
1:A:438:SER:HB3	1:A:566:GLN:HE22	1.82	0.44
1:A:299:TRP:CG	1:A:300:PRO:HA	2.53	0.43
1:A:530:GLU:HG3	1:A:534:GLN:HE21	1.82	0.43
1:A:820:GLU:HA	1:A:820:GLU:OE1	2.17	0.43
1:A:684:ILE:O	1:A:688:GLU:HB2	2.18	0.43
1:A:487:ARG:HG3	6:A:9:GOL:H12	2.01	0.43
1:A:663:LYS:HD2	8:A:70:HOH:O	2.18	0.43
1:A:664:THR:HG23	4:A:1:SSJ:H39A	2.00	0.43
1:A:686:TYR:O	1:A:687:GLU:CB	2.67	0.43
1:A:657:LEU:CD1	1:A:660:ARG:CZ	2.97	0.42
1:A:683:ALA:O	1:A:685:PRO:HD3	2.19	0.42
1:A:646:MET:HE2	1:A:647:PHE:CE2	2.54	0.42
1:A:674:SER:O	1:A:678:LEU:HD13	2.19	0.42
1:A:678:LEU:CD2	1:A:693:ILE:HG13	2.49	0.42
1:A:549:LEU:HB2	1:A:550:PRO:HD3	2.02	0.42
1:A:664:THR:HG21	4:A:1:SSJ:H40B	2.01	0.42
1:A:420:LEU:O	1:A:420:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:LEU:HD21	1:A:693:ILE:CG1	2.49	0.42
1:A:337:GLU:HB3	1:A:340:LYS:HD3	2.01	0.41
1:A:664:THR:CG2	4:A:1:SSJ:C40	2.98	0.41
1:A:670:LEU:O	1:A:670:LEU:HD22	2.20	0.41
1:A:670:LEU:HG	1:A:696:TYR:OH	2.20	0.41
1:A:671:TYR:HD2	3:C:204:DA:C2	2.38	0.41
1:A:337:GLU:CB	1:A:340:LYS:HD3	2.50	0.41
1:A:615:GLU:OE1	4:A:1:SSJ:H2'A	2.21	0.41
1:A:684:ILE:HG22	1:A:685:PRO:O	2.20	0.41
3:C:207:DC:OP2	6:C:1:GOL:H11	2.20	0.41
1:A:659:ARG:NH2	8:A:70:HOH:O	2.54	0.41
1:A:663:LYS:CD	8:A:70:HOH:O	2.68	0.41
1:A:678:LEU:O	1:A:679:SER:C	2.59	0.41
1:A:643:ALA:O	1:A:647:PHE:HD2	2.02	0.41
1:A:771:ARG:O	1:A:774:GLU:HG2	2.21	0.41
1:A:313:ARG:HH22	7:A:12:PGE:H42	1.85	0.41
1:A:642:THR:HG21	1:A:666:ASN:HD21	1.85	0.41
4:A:1:SSJ:O5'	4:A:1:SSJ:H6	2.21	0.40
1:A:526:HIS:CG	1:A:527:PRO:HD2	2.56	0.40
1:A:647:PHE:C	1:A:649:VAL:HG13	2.42	0.40
1:A:650:PRO:HB2	1:A:652:GLU:HG2	2.03	0.40
1:A:535:TYR:CZ	1:A:539:THR:HG21	2.57	0.40
1:A:679:SER:CB	1:A:685:PRO:CG	2.99	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	537/540 (99%)	512 (95%)	22 (4%)	3 (1%)	25 19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	654	VAL
1	A	683	ALA
1	A	586	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	441/441 (100%)	425 (96%)	16 (4%)	35 34

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	LEU
1	A	487	ARG
1	A	519	LEU
1	A	522	LEU
1	A	560	LEU
1	A	612	SER
1	A	651	ARG
1	A	670	LEU
1	A	682	LEU
1	A	686	TYR
1	A	690	GLN
1	A	704	ARG
1	A	711	LEU
1	A	760	LEU
1	A	794	GLU
1	A	805	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	ASN
1	A	534	GLN
1	A	561	HIS

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Mol	Chain	Res	Type
1	A	565	ASN
1	A	566	GLN
1	A	592	GLN
1	A	627	ASN
1	A	639	HIS
1	A	666	ASN
1	A	690	GLN
1	A	754	GLN

### 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	B	112	3,2	14,19,20	2.36	4 (28%)	13,26,29	1.47	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	B	112	3,2	-	0/4/18/19	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	DOC	C6-N1	6.01	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	DOC	O4'-C4'	-3.87	1.37	1.44
2	B	112	DOC	O5'-C5'	-3.27	1.36	1.44
2	B	112	DOC	C2-N3	2.04	1.42	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	112	DOC	C2-N3-C4	3.74	120.13	116.34
2	B	112	DOC	O4'-C1'-C2'	2.90	109.81	106.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	112	DOC	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	GOL	A	4	-	5,5,5	0.34	0	5,5,5	0.28	0
7	PGE	A	10	-	3,3,9	0.42	0	2,2,8	0.32	0
7	PGE	A	7	-	3,3,9	0.42	0	2,2,8	0.31	0
6	GOL	A	15	-	5,5,5	0.40	0	5,5,5	0.11	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PGE	A	11	-	3,3,9	0.41	0	2,2,8	0.33	0
7	PGE	A	13	-	3,3,9	0.44	0	2,2,8	0.11	0
7	PGE	A	8	-	3,3,9	0.41	0	2,2,8	0.29	0
6	GOL	A	9	-	5,5,5	0.32	0	5,5,5	0.53	0
7	PGE	C	2	-	7,7,9	0.43	0	6,6,8	0.38	0
7	PGE	A	16	-	3,3,9	0.41	0	2,2,8	0.32	0
6	GOL	A	5	-	5,5,5	0.38	0	5,5,5	0.20	0
7	PGE	A	17	-	3,3,9	0.42	0	2,2,8	0.30	0
4	SSJ	A	1	5	33,42,42	4.26	4 (12%)	40,68,68	2.13	11 (27%)
7	PGE	A	12	-	5,5,9	0.38	0	4,4,8	0.32	0
6	GOL	A	6	-	5,5,5	0.39	0	5,5,5	0.16	0
7	PGE	A	18	-	3,3,9	0.43	0	2,2,8	0.22	0
6	GOL	C	1	-	5,5,5	0.34	0	5,5,5	0.35	0
7	PGE	A	14	-	3,3,9	0.42	0	2,2,8	0.30	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
6	GOL	A	4	-	-	0/4/4/4	-
7	PGE	A	10	-	-	0/1/1/7	-
7	PGE	A	7	-	-	0/1/1/7	-
6	GOL	A	15	-	-	2/4/4/4	-
7	PGE	A	11	-	-	0/1/1/7	-
7	PGE	A	13	-	-	0/1/1/7	-
7	PGE	A	8	-	-	0/1/1/7	-
6	GOL	A	9	-	-	2/4/4/4	-
7	PGE	C	2	-	-	2/5/5/7	-
7	PGE	A	16	-	-	0/1/1/7	-
6	GOL	A	5	-	-	0/4/4/4	-
7	PGE	A	17	-	-	0/1/1/7	-
4	SSJ	A	1	5	-	7/22/62/62	0/3/3/3
7	PGE	A	12	-	-	1/3/3/7	-
6	GOL	A	6	-	-	4/4/4/4	-
7	PGE	A	18	-	-	0/1/1/7	-
6	GOL	C	1	-	-	2/4/4/4	-
7	PGE	A	14	-	-	1/1/1/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	SSJ	C31-C32	-22.26	1.26	1.43
4	A	1	SSJ	C5-C30	-7.98	1.29	1.43
4	A	1	SSJ	C36-N35	-4.64	1.44	1.50
4	A	1	SSJ	C2-N3	-2.24	1.33	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	SSJ	C4-N3-C2	6.37	120.52	115.14
4	A	1	SSJ	C34-C33-C32	-4.79	109.71	113.55
4	A	1	SSJ	C5-C4-N3	-4.75	121.09	124.40
4	A	1	SSJ	C33-C34-N35	3.84	102.33	99.37
4	A	1	SSJ	C32-C36-N35	3.46	101.97	99.21
4	A	1	SSJ	C37-C34-C33	-3.40	109.32	112.79
4	A	1	SSJ	C6-C5-C30	3.34	123.50	118.69
4	A	1	SSJ	C2'-C1'-N1	-3.17	106.96	114.27
4	A	1	SSJ	PB-O3A-PA	-2.37	124.69	132.83
4	A	1	SSJ	PB-O3B-PG	-2.27	125.05	132.83
4	A	1	SSJ	C37-C34-N35	2.23	112.85	110.00

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	15	GOL	O1-C1-C2-C3
6	A	9	GOL	O1-C1-C2-C3
4	A	1	SSJ	C5'-O5'-PA-O2A
4	A	1	SSJ	PB-O3B-PG-O1G
6	A	9	GOL	O1-C1-C2-O2
6	A	6	GOL	O1-C1-C2-C3
6	A	6	GOL	C1-C2-C3-O3
6	C	1	GOL	O1-C1-C2-C3
6	A	6	GOL	O2-C2-C3-O3
6	C	1	GOL	O1-C1-C2-O2
7	A	14	PGE	O2-C3-C4-O3
4	A	1	SSJ	C5-C30-C31-C32
6	A	15	GOL	O1-C1-C2-O2
4	A	1	SSJ	C5'-O5'-PA-O3A
7	C	2	PGE	C3-C4-O3-C5
4	A	1	SSJ	PA-O3A-PB-O1B
4	A	1	SSJ	C5'-O5'-PA-O1A
6	A	6	GOL	O1-C1-C2-O2

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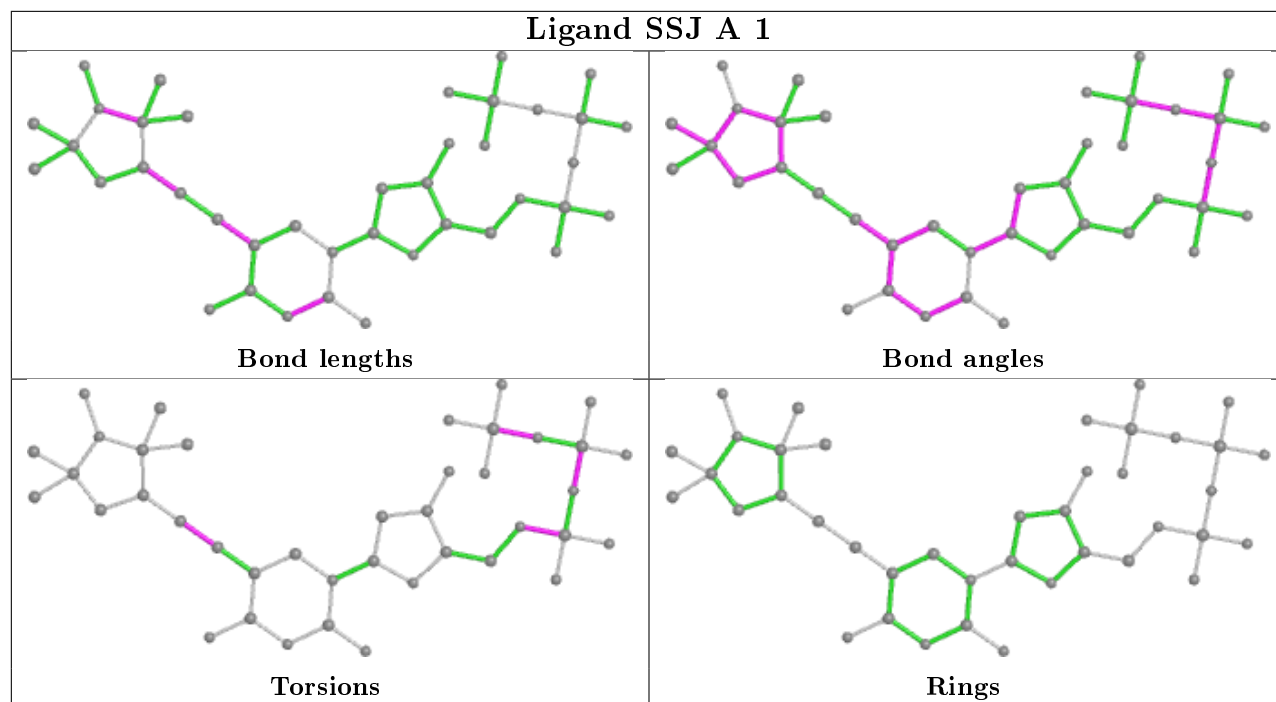
Mol	Chain	Res	Type	Atoms
7	A	12	PGE	O2-C3-C4-O3
4	A	1	SSJ	PB-O3B-PG-O3G
7	C	2	PGE	O2-C3-C4-O3

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	9	GOL	1	0
7	C	2	PGE	4	0
4	A	1	SSJ	10	0
7	A	12	PGE	1	0
6	A	6	GOL	1	0
6	C	1	GOL	2	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	539/540 (99%)	0.21	40 (7%) 14 13	20, 36, 100, 177	0
2	B	11/12 (91%)	-0.37	0 100 100	25, 29, 58, 63	0
3	C	14/16 (87%)	-0.11	1 (7%) 16 15	24, 32, 58, 110	0
All	All	564/568 (99%)	0.19	41 (7%) 15 14	20, 36, 98, 177	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	692	PHE	8.5
1	A	682	LEU	6.7
1	A	647	PHE	6.2
1	A	648	GLY	6.0
1	A	691	ALA	5.9
1	A	645	TRP	5.5
1	A	696	TYR	5.1
1	A	678	LEU	5.0
1	A	688	GLU	4.8
1	A	649	VAL	4.8
1	A	657	LEU	4.7
1	A	654	VAL	4.6
1	A	690	GLN	4.5
1	A	644	SER	4.4
1	A	661	ALA	4.0
1	A	687	GLU	3.7
1	A	646	MET	3.7
1	A	640	THR	3.7
1	A	650	PRO	3.5
1	A	653	ALA	3.4
1	A	656	PRO	3.4
1	A	658	MET	3.2
1	A	664	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	300	PRO	3.1
1	A	684	ILE	3.0
1	A	689	ALA	3.0
1	A	695	ARG	2.9
1	A	665	ILE	2.9
1	A	693	ILE	2.9
1	A	655	ASP	2.9
1	A	652	GLU	2.7
1	A	669	VAL	2.7
1	A	697	PHE	2.6
1	A	679	SER	2.5
1	A	299	TRP	2.5
1	A	642	THR	2.4
1	A	676	HIS	2.4
1	A	651	ARG	2.4
1	A	680	GLN	2.3
3	C	203	DA	2.2
1	A	461	LEU	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	B	112	18/19	0.97	0.12	27,35,43,55	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

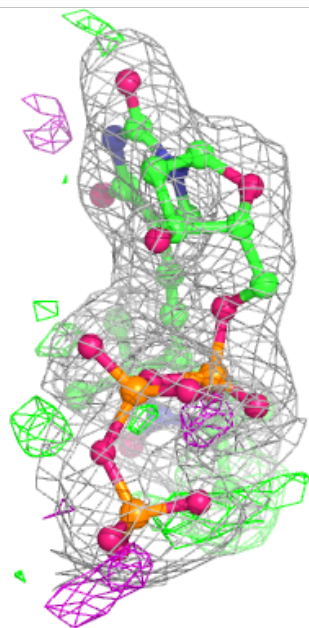
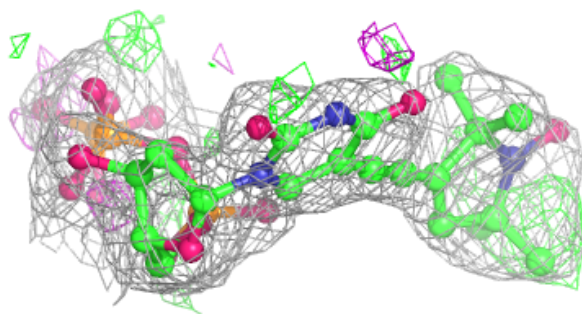
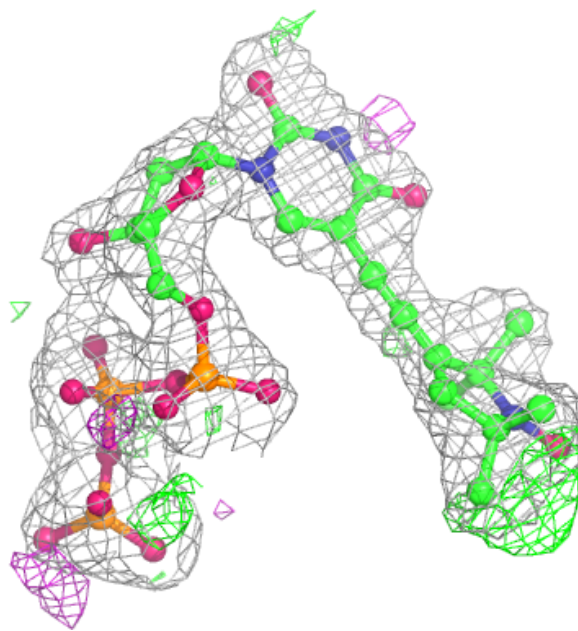
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	PGE	A	14	4/10	0.68	0.23	61,72,79,79	0
7	PGE	A	16	4/10	0.69	0.17	47,58,69,69	0
7	PGE	A	10	4/10	0.72	0.23	46,67,75,75	0
7	PGE	A	12	6/10	0.74	0.22	49,57,68,68	0
7	PGE	A	11	4/10	0.79	0.21	42,58,70,70	0
6	GOL	A	9	6/6	0.82	0.28	42,58,69,75	0
6	GOL	A	15	6/6	0.83	0.18	50,62,71,77	0
7	PGE	C	2	8/10	0.88	0.22	32,54,61,61	0
7	PGE	A	17	4/10	0.88	0.10	58,60,73,73	0
7	PGE	A	18	4/10	0.89	0.11	58,61,73,73	0
7	PGE	A	13	4/10	0.90	0.13	48,52,63,63	0
6	GOL	A	6	6/6	0.93	0.14	40,48,54,59	0
6	GOL	A	4	6/6	0.93	0.12	30,36,42,49	0
6	GOL	C	1	6/6	0.93	0.17	43,58,72,72	0
5	MG	A	3	1/1	0.93	0.22	59,59,59,59	0
7	PGE	A	8	4/10	0.94	0.10	40,53,59,59	0
4	SSJ	A	1	40/40	0.94	0.13	29,44,60,128	0
7	PGE	A	7	4/10	0.96	0.12	35,52,66,66	0
6	GOL	A	5	6/6	0.96	0.09	22,27,31,38	0
5	MG	A	2	1/1	0.99	0.10	27,27,27,27	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 SSJ A 1:**

$2mF_o-DF_c$  (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.