



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 11:39 PM EDT

PDB ID : 3OJU / pdb_00003oju
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

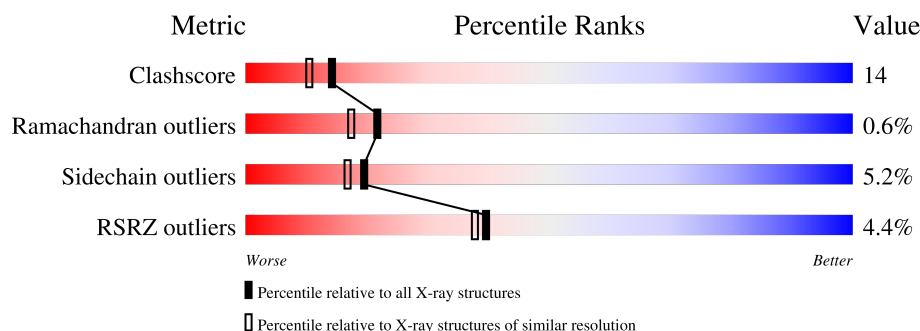
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 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 $\leq 5\%$. 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>5%</div> <div> <div>74%</div> <div>24%</div> <div>.</div> </div> </div>
2	B	12	<div> <div>75%</div> <div>17%</div> <div>8%</div> </div>
3	C	16	<div> <div>44%</div> <div>44%</div> <div>12%</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			

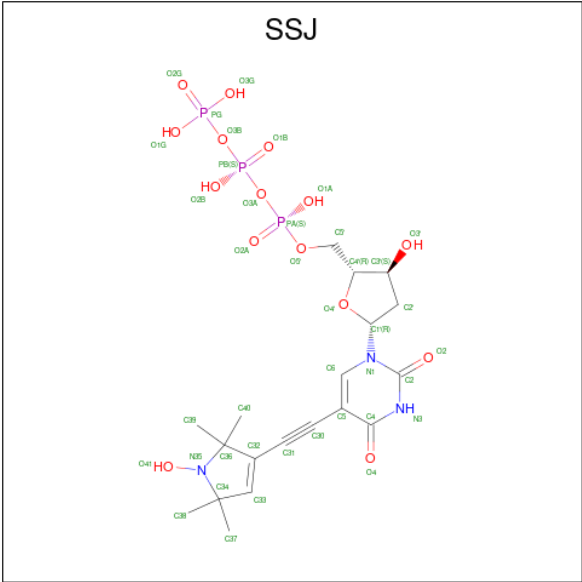
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*CP*(DOC))-3').

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) (CCD ID: SSJ) (formula: C₁₉H₂₈N₃O₁₅P₃).

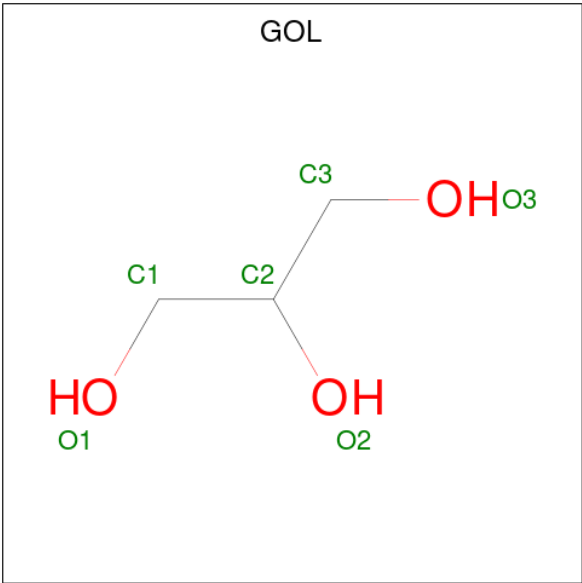


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			40	19	3	15	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

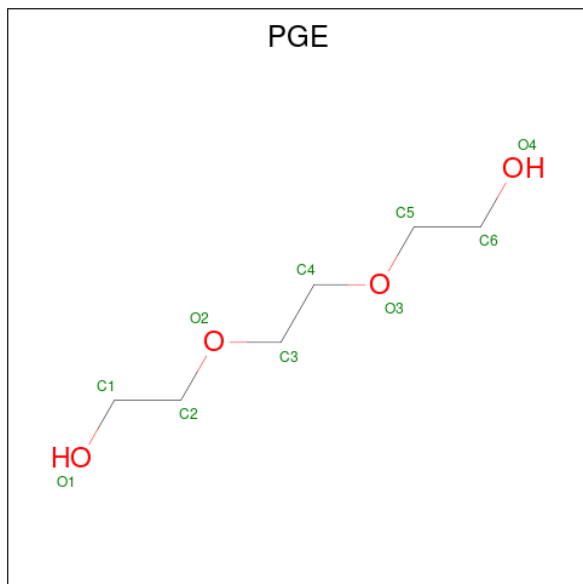
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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 (CCD ID: 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		

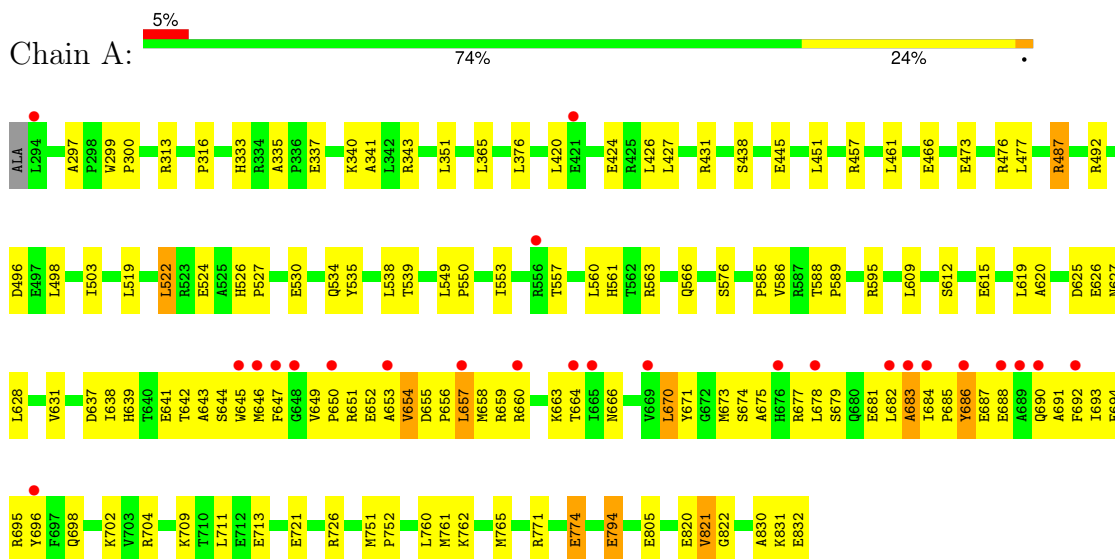
- Molecule 8 is water.

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		

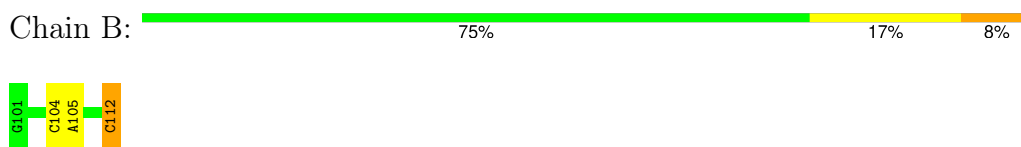
3 Residue-property plots [i](#)

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

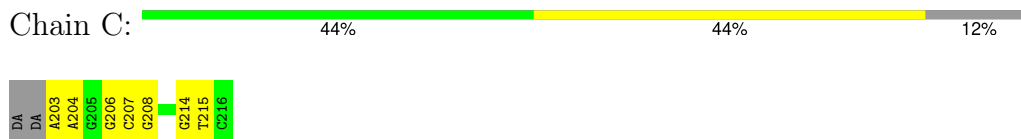
- Molecule 1: DNA polymerase I, thermostable



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.177 , 0.219 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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.

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: PGE, GOL, DOC, MG, SSJ

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	0.36	0/4376	0.73	1/5927 (0.0%)
2	B	0.14	0/249	0.72	0/382
3	C	0.17	0/325	0.65	0/500
All	All	0.34	0/4950	0.73	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($^{\circ}$)	Ideal($^{\circ}$)
1	A	498	LEU	N-CA-C	-5.24	103.61	110.53

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	123	0
2	B	240	12	134	2	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	136	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 (136) 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:762:LYS:HA	1:A:765:MET:HE3	1.61	0.82
1:A:664:THR:HG21	4:A:1:SSJ:H40	1.66	0.75
1:A:343:ARG:NH1	1:A:365:LEU:HD11	2.04	0.73
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:794:GLU:H	1:A:794:GLU:CD	2.07	0.63
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:664:THR:HG23	4:A:1:SSJ:H39B	1.82	0.61
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:761:MET:HG3	1:A:765:MET:HE2	1.82	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:615:GLU:CD	4:A:1:SSJ:H2'A	2.29	0.58
1:A:625:ASP:HB2	1:A:702:LYS:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:686:TYR:C	1:A:688:GLU:H	2.14	0.54
3:C:207:DC:OP2	7:C:2:PGE:H6	2.07	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:664:THR:CG2	4:A:1:SSJ:H40	2.36	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:626:GLU:H	1:A:626:GLU:CD	2.18	0.51
1:A:673:MET:HE2	1:A:677:ARG:HG2	1.93	0.51
1:A:831:LYS:O	1:A:832:GLU:HB2	2.10	0.51
1:A:659:ARG:HD3	8:A:53:HOH:O	2.10	0.51
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:445:GLU:O	1:A:561:HIS:HD2	1.98	0.47
1:A:679:SER:HB2	1:A:685:PRO:CG	2.45	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:673:MET:HE1	1:A:681:GLU:HG3	1.97	0.46
1:A:678:LEU:O	1:A:679:SER:C	2.59	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:647:PHE:C	1:A:649:VAL:HG13	2.42	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:664:THR:HG21	4:A:1:SSJ:C40	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:PHE:C	1:A:692:PHE:CD2	2.98	0.42
1:A:549:LEU:HB2	1:A:550:PRO:HD3	2.02	0.42
1:A:420:LEU:O	1:A:420:LEU:HG	2.19	0.42
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:HD22	1:A:670:LEU:O	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: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
1:A:653:ALA:C	1:A:654:VAL:HG23	2.46	0.41
1:A:664:THR:CG2	4:A:1:SSJ:H39B	2.50	0.41
1:A:526:HIS:CG	1:A:527:PRO:HD2	2.56	0.40
4:A:1:SSJ:H6	4:A:1:SSJ:O5'	2.21	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

5.3.1 Protein backbone

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%)	22	17

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	441/441 (100%)	418 (95%)	23 (5%)	19	17

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	LEU
1	A	424	GLU
1	A	487	ARG
1	A	519	LEU
1	A	522	LEU
1	A	524	GLU
1	A	560	LEU
1	A	612	SER
1	A	651	ARG
1	A	657	LEU
1	A	670	LEU
1	A	682	LEU
1	A	686	TYR
1	A	690	GLN
1	A	704	ARG
1	A	709	LYS
1	A	711	LEU
1	A	713	GLU

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Mol	Chain	Res	Type
1	A	760	LEU
1	A	774	GLU
1	A	794	GLU
1	A	805	GLU
1	A	821	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	534	GLN
1	A	561	HIS
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	750	ASN
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	2,3	16,19,20	2.48	7 (43%)	20,26,29	1.14	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	B	112	2,3	-	0/7/18/19	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	DOC	O2-C2	6.46	1.35	1.23
2	B	112	DOC	O4'-C4'	-4.04	1.37	1.44
2	B	112	DOC	C2-N3	2.96	1.42	1.36
2	B	112	DOC	C4-N4	2.88	1.40	1.33
2	B	112	DOC	O5'-C5'	-2.54	1.36	1.44
2	B	112	DOC	C6-C5	2.28	1.40	1.35
2	B	112	DOC	C6-N1	2.17	1.43	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	112	DOC	O4'-C1'-C2'	2.87	109.81	106.41
2	B	112	DOC	C1'-N1-C2	2.13	121.48	117.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	112	DOC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
7	PGE	A	14	-	3,3,9	0.38	0	2,2,8	0.35	0
4	SSJ	A	1	5	39,42,42	3.99	9 (23%)	55,68,68	2.06	13 (23%)
7	PGE	A	8	-	3,3,9	0.37	0	2,2,8	0.34	0
7	PGE	A	16	-	3,3,9	0.38	0	2,2,8	0.37	0
7	PGE	A	13	-	3,3,9	0.40	0	2,2,8	0.17	0
7	PGE	A	7	-	3,3,9	0.38	0	2,2,8	0.35	0
7	PGE	A	12	-	5,5,9	0.38	0	4,4,8	0.32	0
7	PGE	A	11	-	3,3,9	0.37	0	2,2,8	0.38	0
6	GOL	A	4	-	5,5,5	0.34	0	5,5,5	0.31	0
7	PGE	A	17	-	3,3,9	0.38	0	2,2,8	0.35	0
6	GOL	C	1	-	5,5,5	0.34	0	5,5,5	0.38	0
7	PGE	C	2	-	7,7,9	0.43	0	6,6,8	0.37	0
7	PGE	A	18	-	3,3,9	0.39	0	2,2,8	0.27	0
6	GOL	A	9	-	5,5,5	0.33	0	5,5,5	0.57	0
6	GOL	A	5	-	5,5,5	0.38	0	5,5,5	0.24	0
6	GOL	A	6	-	5,5,5	0.40	0	5,5,5	0.18	0
7	PGE	A	10	-	3,3,9	0.38	0	2,2,8	0.37	0
6	GOL	A	15	-	5,5,5	0.41	0	5,5,5	0.14	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
7	PGE	A	14	-	-	1/1/1/7	-
4	SSJ	A	1	5	-	8/23/62/62	0/3/3/3
7	PGE	A	8	-	-	0/1/1/7	-
7	PGE	A	16	-	-	0/1/1/7	-
7	PGE	A	13	-	-	0/1/1/7	-
7	PGE	A	7	-	-	0/1/1/7	-
7	PGE	A	12	-	-	1/3/3/7	-
7	PGE	A	11	-	-	0/1/1/7	-
6	GOL	A	4	-	-	0/4/4/4	-
7	PGE	A	17	-	-	0/1/1/7	-
6	GOL	C	1	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGE	C	2	-	-	2/5/5/7	-
7	PGE	A	18	-	-	0/1/1/7	-
6	GOL	A	9	-	-	2/4/4/4	-
6	GOL	A	5	-	-	0/4/4/4	-
6	GOL	A	6	-	-	4/4/4/4	-
7	PGE	A	10	-	-	0/1/1/7	-
6	GOL	A	15	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	SSJ	C31-C32	-22.09	1.26	1.43
4	A	1	SSJ	C30-C5	-6.75	1.29	1.43
4	A	1	SSJ	C36-N35	-4.86	1.44	1.50
4	A	1	SSJ	C5-C4	-3.43	1.39	1.44
4	A	1	SSJ	PB-O3A	2.64	1.62	1.59
4	A	1	SSJ	PB-O3B	2.62	1.62	1.59
4	A	1	SSJ	C4-N3	-2.48	1.34	1.38
4	A	1	SSJ	C2-N3	-2.44	1.33	1.38
4	A	1	SSJ	PA-O3A	2.33	1.62	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	SSJ	C5-C4-N3	6.23	121.09	114.14
4	A	1	SSJ	C4-N3-C2	-5.20	120.52	127.34
4	A	1	SSJ	C34-C33-C32	-4.88	109.71	113.45
4	A	1	SSJ	C33-C34-N35	4.21	102.33	99.43
4	A	1	SSJ	O4-C4-C5	-4.17	119.99	125.12
4	A	1	SSJ	C32-C36-N35	3.82	101.97	99.18
4	A	1	SSJ	N3-C2-N1	3.81	119.85	114.89
4	A	1	SSJ	C37-C34-C33	-3.63	109.32	112.77
4	A	1	SSJ	O4'-C1'-N1	3.02	113.22	107.86
4	A	1	SSJ	C5-C6-N1	-3.00	118.68	122.04
4	A	1	SSJ	C2'-C1'-N1	-2.74	106.96	113.81
4	A	1	SSJ	C37-C34-N35	2.45	112.85	110.05
4	A	1	SSJ	O2-C2-N1	-2.22	119.90	122.80

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	SSJ	C5'-O5'-PA-O2A
4	A	1	SSJ	C5'-O5'-PA-O3A
4	A	1	SSJ	PB-O3B-PG-O1G
6	A	9	GOL	O1-C1-C2-C3
6	A	15	GOL	O1-C1-C2-C3
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
6	A	15	GOL	O1-C1-C2-O2
7	A	14	PGE	O2-C3-C4-O3
7	C	2	PGE	C3-C4-O3-C5
4	A	1	SSJ	PA-O3A-PB-O1B
4	A	1	SSJ	C5-C30-C31-C32
4	A	1	SSJ	C5'-O5'-PA-O1A
6	A	6	GOL	O1-C1-C2-O2
4	A	1	SSJ	PB-O3B-PG-O3G
7	A	12	PGE	O2-C3-C4-O3
7	C	2	PGE	O2-C3-C4-O3
4	A	1	SSJ	PA-O3A-PB-O2B

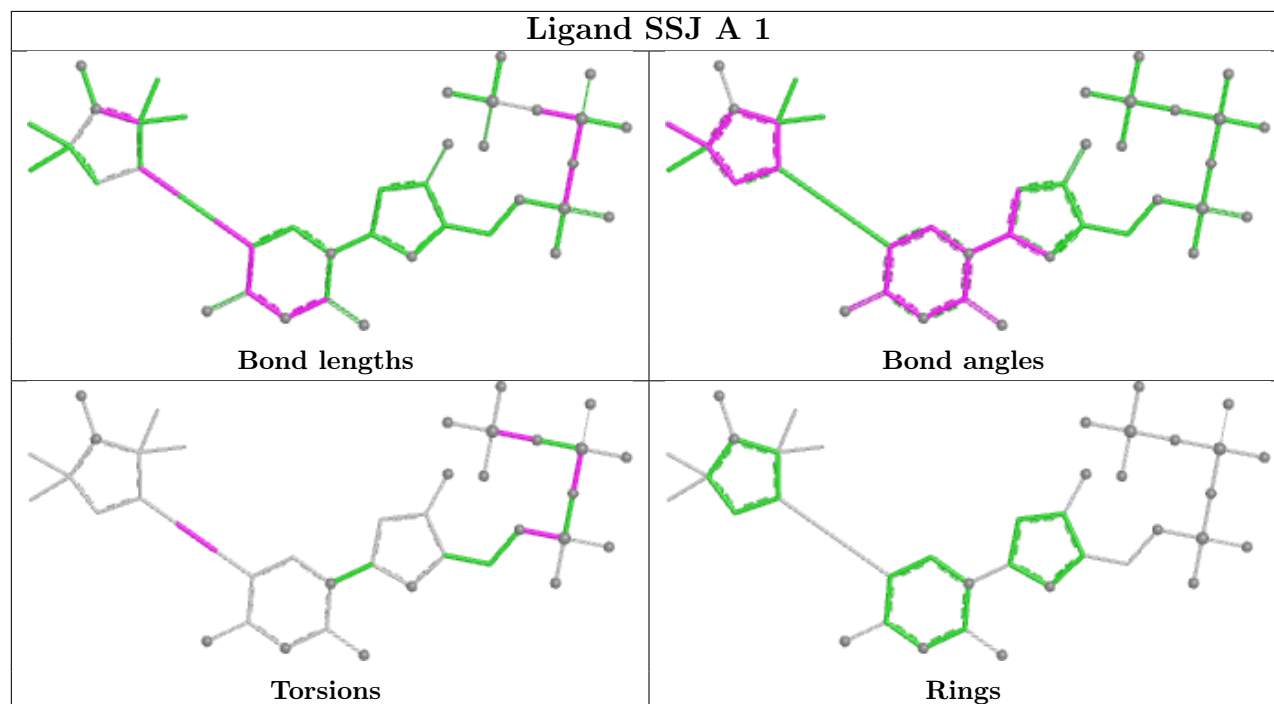
There are no ring outliers.

6 monomers are involved in 18 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [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, 95th 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 ²)	Q<0.9
1	A	539/540 (99%)	-0.14	25 (4%) 38 36	22, 40, 109, 190	0
2	B	11/12 (91%)	-0.61	0 100 100	25, 29, 58, 63	0
3	C	14/16 (87%)	-0.44	0 100 100	24, 32, 58, 110	0
All	All	564/568 (99%)	-0.16	25 (4%) 39 38	22, 40, 108, 190	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	684	ILE	4.7
1	A	645	TRP	4.2
1	A	686	TYR	4.2
1	A	692	PHE	3.9
1	A	665	ILE	3.6
1	A	676	HIS	3.3
1	A	648	GLY	3.2
1	A	683	ALA	3.1
1	A	657	LEU	2.9
1	A	696	TYR	2.8
1	A	690	GLN	2.8
1	A	650	PRO	2.6
1	A	682	LEU	2.6
1	A	689	ALA	2.5
1	A	647	PHE	2.3
1	A	294	LEU	2.3
1	A	421	GLU	2.2
1	A	653	ALA	2.2
1	A	660	ARG	2.1
1	A	556	ARG	2.1
1	A	678	LEU	2.1
1	A	669	VAL	2.1
1	A	646	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	664	THR	2.0
1	A	688	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, 95th 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	DOC	B	112	18/19	0.95	0.07	27,35,43,55	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, 95th 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
7	PGE	A	17	4/10	0.74	0.14	58,60,73,73	0
7	PGE	A	16	4/10	0.76	0.16	47,58,69,69	0
7	PGE	A	10	4/10	0.77	0.19	46,67,75,75	0
7	PGE	A	14	4/10	0.78	0.17	61,72,79,79	0
7	PGE	A	12	6/10	0.80	0.22	49,57,68,68	0
6	GOL	A	9	6/6	0.85	0.12	42,58,69,75	0
7	PGE	A	11	4/10	0.85	0.13	42,58,70,70	0
6	GOL	A	15	6/6	0.85	0.12	50,62,71,77	0
7	PGE	C	2	8/10	0.87	0.14	32,54,61,61	0
6	GOL	C	1	6/6	0.88	0.11	43,58,72,72	0
5	MG	A	3	1/1	0.88	0.21	59,59,59,59	0
7	PGE	A	7	4/10	0.89	0.10	35,52,66,66	0
4	SSJ	A	1	40/40	0.90	0.12	29,44,60,128	0
7	PGE	A	13	4/10	0.90	0.12	48,52,63,63	0
7	PGE	A	18	4/10	0.90	0.16	58,61,73,73	0

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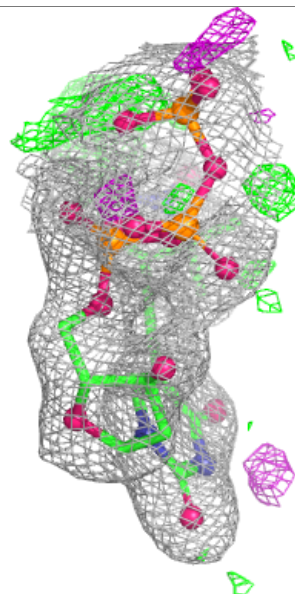
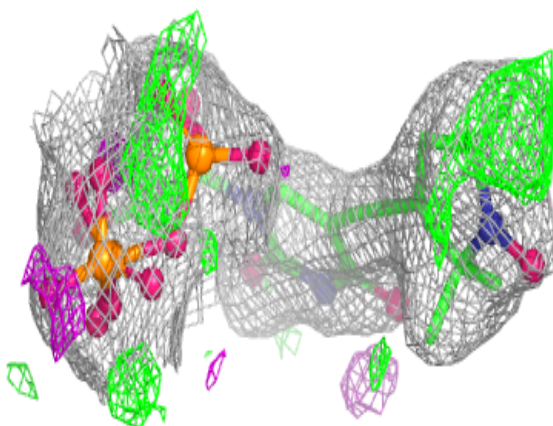
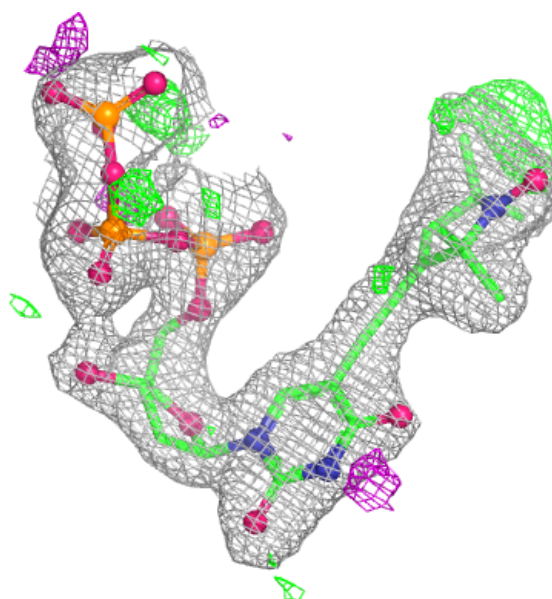
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	A	6	6/6	0.90	0.10	40,48,54,59	0
6	GOL	A	4	6/6	0.92	0.11	30,36,42,49	0
7	PGE	A	8	4/10	0.93	0.09	40,53,59,59	0
6	GOL	A	5	6/6	0.95	0.06	22,27,31,38	0
5	MG	A	2	1/1	0.99	0.01	27,27,27,27	0

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.