



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:08 pm BST

PDB ID : 3OJS
Title : Snapshots of the large fragment of DNA polymerase I from *Thermus Aquaticus* processing C5 modified thymidines
Authors : Marx, A.; Diederichs, K.; Obeid, S.
Deposited on : 2010-08-23
Resolution : 1.90 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 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

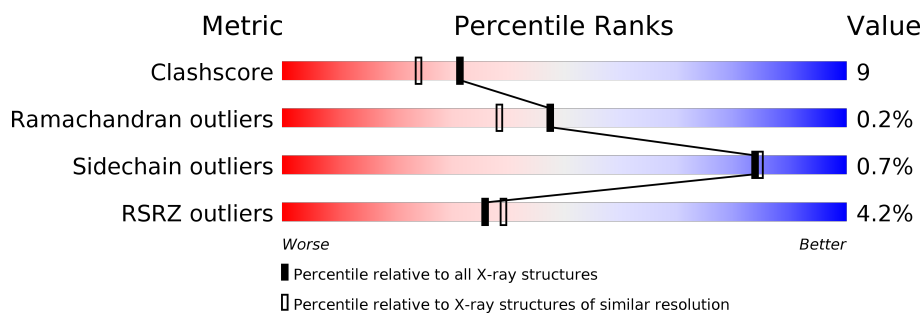
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 ≥ 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>4%</div> <div>87%</div> <div>13%</div> </div>
2	B	12	<div> <div>8%</div> <div>83%</div> <div>8%</div> </div>
3	C	16	<div> <div>31%</div> <div>50%</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	XJS	A	1	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	2	-	-	X	-
5	GOL	B	7	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9792 atoms, of which 4446 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	2	0
			8643	2732	4345	772	781	13			

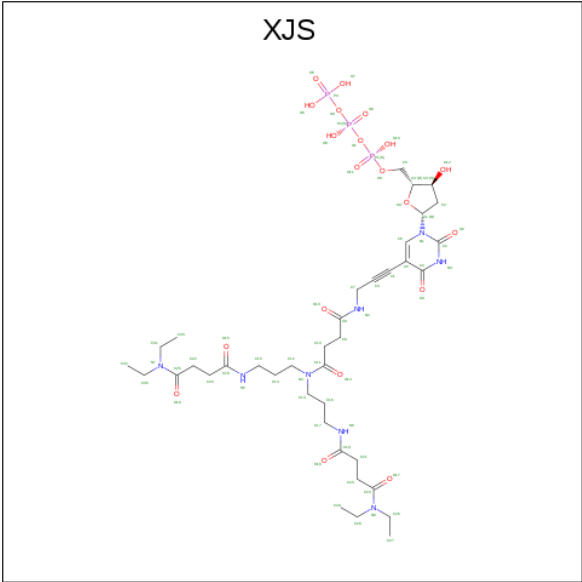
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*CP*(DOC))-3').

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').

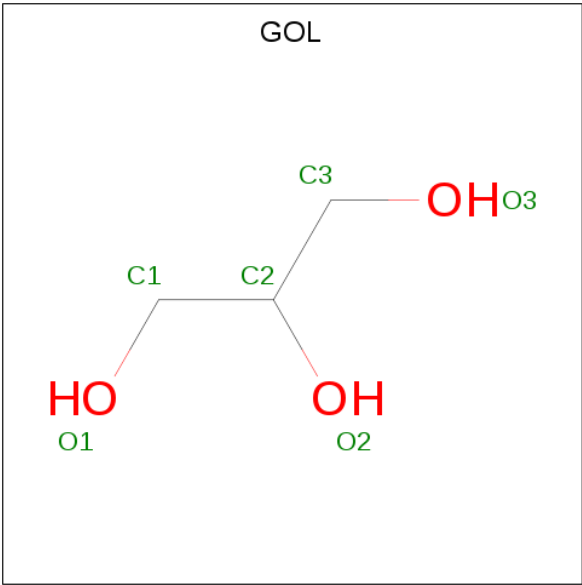
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	P	0	0	0
			329	156	66	92	15			

- Molecule 4 is 2'-deoxy-5-[9-(3-{[4-(diethylamino)-4-oxobutanoyl]amino}propyl)-18-ethyl-5,8,14,17-tetraoxo-4,9,13,18-tetraazaicos-1-yn-1-yl]uridine 5'-(tetrahydrogen triphosphate) (three-letter code: XJS) (formula: C₃₈H₆₃N₈O₂₀P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			69	38	8	20	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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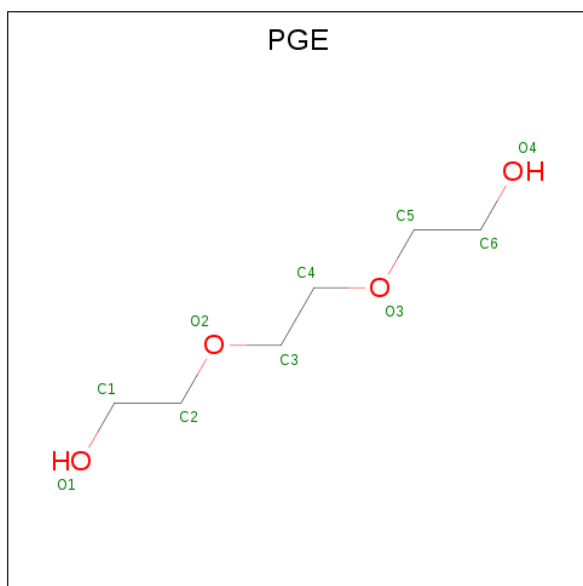
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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		

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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

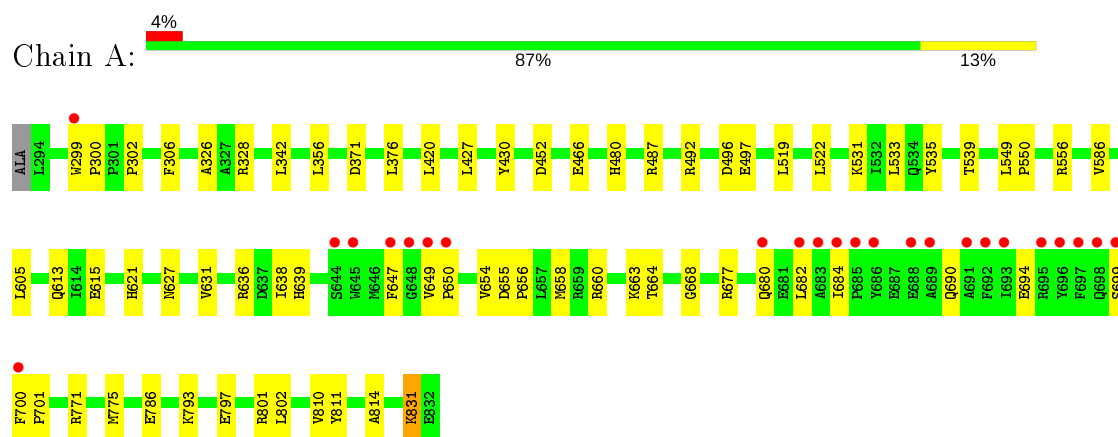
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	275	Total	O	0	0
			275	275		
9	B	22	Total	O	0	0
			22	22		
9	C	34	Total	O	0	0
			34	34		

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, α , β , γ	107.83 Å 107.83 Å 90.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.69 – 1.90 46.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.69-1.90) 99.0 (46.69-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.90 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.163 , 0.212 0.165 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9792	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 3.76% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, PGE, DOC, XJS, ACT

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	0.33	0/4394	0.50	0/5950
2	B	0.80	0/249	1.45	4/382 (1.0%)
3	C	0.69	0/370	1.35	5/570 (0.9%)
All	All	0.40	0/5013	0.69	9/6902 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	DC	O4'-C1'-N1	7.28	113.09	108.00
3	C	212	DT	O4'-C1'-N1	-7.00	103.10	108.00
3	C	208	DG	O4'-C1'-N9	-6.63	103.36	108.00
2	B	108	DG	O4'-C1'-N9	6.55	112.59	108.00
3	C	206	DG	O4'-C4'-C3'	-6.37	101.95	104.50
2	B	108	DG	C1'-O4'-C4'	-6.21	103.89	110.10
3	C	210	DC	O4'-C1'-C2'	5.61	110.38	105.90
3	C	209	DC	O4'-C1'-N1	-5.27	104.31	108.00
2	B	106	DC	O4'-C1'-N1	-5.16	104.39	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4298	4345	4355	49	0
2	B	240	12	134	12	0
3	C	329	0	180	18	0
4	A	69	0	59	22	0
5	A	30	40	40	6	0
5	B	6	8	8	4	0
5	C	12	16	16	1	0
6	A	2	0	0	0	0
7	A	12	12	12	1	0
7	C	5	4	4	1	0
8	A	12	9	9	1	0
9	A	275	0	0	3	0
9	B	22	0	0	1	0
9	C	34	0	0	1	0
All	All	5346	4446	4817	88	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 9.

All (88) 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)
4:A:1:XJS:H27A	4:A:1:XJS:H23A	1.31	1.12
3:C:214:DG:H2''	3:C:215:DT:H5''	1.23	1.10
4:A:1:XJS:H22	4:A:1:XJS:H63	1.25	1.10
3:C:214:DG:C2'	3:C:215:DT:H5''	2.04	0.86
4:A:1:XJS:H22	4:A:1:XJS:C33	2.03	0.82
2:B:103:DC:H2''	2:B:104:DC:H5'	1.63	0.81
4:A:1:XJS:C27	4:A:1:XJS:H23A	2.13	0.79
3:C:209:DC:H3'	7:C:6:PGE:H4	1.65	0.77
1:A:680:GLN:HG3	3:C:202:DA:H2	1.50	0.75
3:C:214:DG:H2''	3:C:215:DT:C5'	2.12	0.70
5:A:2:GOL:H32	3:C:212:DT:H4'	1.75	0.67
4:A:1:XJS:C22	4:A:1:XJS:H63	2.14	0.66
4:A:1:XJS:H20	3:C:205:DG:N7	2.11	0.66
4:A:1:XJS:H27A	4:A:1:XJS:C23	2.20	0.65
2:B:104:DC:H2''	2:B:105:DA:H5'	1.81	0.63
2:B:103:DC:H2''	2:B:104:DC:C5'	2.27	0.62
1:A:299:TRP:CG	1:A:300:PRO:HA	2.34	0.62
5:A:2:GOL:C3	3:C:212:DT:H4'	2.29	0.62
1:A:466[B]:GLU:HG3	7:A:835:PGE:H32	1.82	0.62
4:A:1:XJS:H30	3:C:204:DA:H5''	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:GLU:CD	4:A:1:XJS:H2'A	2.22	0.60
5:A:2:GOL:H31	3:C:212:DT:O4'	2.02	0.59
3:C:210:DC:H2'	3:C:211:DG:C8	2.37	0.59
1:A:660:ARG:HH22	4:A:1:XJS:H7	1.68	0.59
1:A:302:PRO:HG2	1:A:328:ARG:HD3	1.86	0.58
1:A:663[B]:LYS:HD2	4:A:1:XJS:C7	2.33	0.58
1:A:639:HIS:CG	1:A:663[A]:LYS:HG2	2.39	0.57
1:A:786:GLU:OE2	1:A:831:LYS:HE2	2.05	0.57
1:A:647:PHE:CD2	1:A:658:MET:HE3	2.40	0.55
1:A:549:LEU:HB2	1:A:550:PRO:HD3	1.89	0.55
5:B:7:GOL:H12	9:B:30:HOH:O	2.08	0.54
4:A:1:XJS:H22A	5:C:8:GOL:O3	2.07	0.54
1:A:660:ARG:NH2	4:A:1:XJS:C7	2.71	0.53
1:A:342:LEU:HD21	1:A:356:LEU:HD11	1.90	0.53
1:A:660:ARG:NH2	4:A:1:XJS:H7	2.23	0.53
1:A:664:THR:HG22	9:A:281:HOH:O	2.09	0.52
4:A:1:XJS:C30	3:C:204:DA:H5''	2.39	0.51
2:B:104:DC:H2''	2:B:105:DA:C5'	2.40	0.51
1:A:420:LEU:O	1:A:427:LEU:CD1	2.58	0.51
2:B:103:DC:H2'	2:B:104:DC:C6	2.46	0.51
5:A:2:GOL:C3	3:C:212:DT:C4'	2.89	0.51
4:A:1:XJS:O18	3:C:204:DA:C8	2.63	0.50
2:B:101:DG:H2''	2:B:102:DA:H5'	1.94	0.50
1:A:480:HIS:HE1	1:A:497:GLU:OE1	1.95	0.50
1:A:420:LEU:O	1:A:427:LEU:HD11	2.12	0.49
1:A:680:GLN:HG3	3:C:202:DA:C2	2.38	0.49
2:B:111:DC:H2'	2:B:112:DOC:H6	1.94	0.49
1:A:631:VAL:HG11	1:A:638:ILE:HD11	1.94	0.49
5:A:2:GOL:H31	3:C:212:DT:C4'	2.42	0.49
4:A:1:XJS:H32	9:C:42:HOH:O	2.12	0.49
1:A:699:SER:C	1:A:701:PRO:HD3	2.33	0.48
2:B:107:DG:O6	5:B:7:GOL:H32	2.13	0.48
2:B:104:DC:H2'	2:B:105:DA:C8	2.49	0.48
1:A:797:GLU:HG3	1:A:801:ARG:NH1	2.29	0.47
2:B:101:DG:H2'	2:B:102:DA:C8	2.48	0.47
1:A:631:VAL:HG13	1:A:636:ARG:HB2	1.95	0.47
1:A:452:ASP:OD2	5:A:3:GOL:H32	2.14	0.47
1:A:810:VAL:HG13	1:A:811:TYR:N	2.29	0.47
1:A:627:ASN:O	1:A:631:VAL:HG23	2.15	0.47
1:A:621:HIS:HD2	1:A:814:ALA:H	1.63	0.46
4:A:1:XJS:H16A	4:A:1:XJS:H12	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:VAL:HA	1:A:658:MET:HE2	1.96	0.46
1:A:556:ARG:HG3	9:A:256:HOH:O	2.15	0.46
1:A:771:ARG:O	1:A:775:MET:HG3	2.16	0.46
1:A:655:ASP:HB2	1:A:656:PRO:HD2	1.98	0.46
1:A:306:PHE:O	1:A:326:ALA:HA	2.15	0.46
1:A:690:GLN:O	1:A:694:GLU:HG3	2.17	0.45
1:A:605:LEU:HG	1:A:793:LYS:HG2	1.99	0.45
1:A:682:LEU:HB2	1:A:684:ILE:HG12	1.99	0.45
1:A:376:LEU:HD22	1:A:420:LEU:HD12	2.00	0.44
1:A:535:TYR:CZ	1:A:539:THR:HG21	2.53	0.44
4:A:1:XJS:H30	3:C:204:DA:C5'	2.47	0.44
2:B:106:DC:C5	5:B:7:GOL:H31	2.53	0.44
1:A:677:ARG:NH1	4:A:1:XJS:H60	2.32	0.43
4:A:1:XJS:H20A	4:A:1:XJS:H15A	1.78	0.43
1:A:649:VAL:HG23	1:A:650:PRO:O	2.19	0.43
1:A:492:ARG:O	1:A:496:ASP:HB2	2.19	0.42
1:A:668:GLY:HA2	3:C:204:DA:C4	2.54	0.42
1:A:519:LEU:HB2	1:A:533:LEU:HD21	2.02	0.42
1:A:621:HIS:CD2	1:A:814:ALA:H	2.38	0.42
1:A:690:GLN:HA	1:A:690:GLN:OE1	2.20	0.41
1:A:802:LEU:C	1:A:802:LEU:HD13	2.41	0.41
1:A:613:GLN:HA	4:A:1:XJS:O8	2.21	0.41
8:A:840:ACT:CH3	9:A:235:HOH:O	2.69	0.41
2:B:107:DG:O6	5:B:7:GOL:C3	2.69	0.40
1:A:531:LYS:HD3	1:A:531:LYS:HA	1.96	0.40
1:A:371:ASP:HA	1:A:430:TYR:OH	2.22	0.40
1:A:700:PHE:N	1:A:701:PRO:HD3	2.36	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	539/540 (100%)	522 (97%)	16 (3%)	1 (0%)	47 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	443/441 (100%)	440 (99%)	3 (1%)	84 84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	487	ARG
1	A	522	LEU
1	A	831	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	ASN
1	A	480	HIS
1	A	485	ASN
1	A	565	ASN
1	A	613	GLN
1	A	621	HIS
1	A	639	HIS
1	A	666	ASN
1	A	676	HIS

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	2.22	5 (35%)	13,26,29	1.69	3 (23%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	DOC	C6-N1	5.23	1.42	1.35
2	B	112	DOC	O4'-C4'	-3.74	1.37	1.44
2	B	112	DOC	C4-N4	2.79	1.43	1.35
2	B	112	DOC	O4'-C1'	-2.46	1.36	1.42
2	B	112	DOC	O5'-C5'	-2.16	1.39	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	112	DOC	C2-N3-C4	3.40	119.79	116.34
2	B	112	DOC	C3'-C2'-C1'	-3.21	99.06	102.78
2	B	112	DOC	C2'-C3'-C4'	-3.11	96.90	102.72

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	838	-	3,3,9	0.34	0	2,2,8	0.55	0
4	XJS	A	1	6	63,70,70	2.75	22 (34%)	77,96,96	1.87	16 (20%)
5	GOL	A	3	-	5,5,5	0.33	0	5,5,5	0.39	0
8	ACT	A	836	-	1,3,3	1.21	0	0,3,3	0.00	-
5	GOL	A	4	-	5,5,5	0.30	0	5,5,5	0.28	0
7	PGE	A	837	-	3,3,9	0.43	0	2,2,8	0.25	0
5	GOL	C	9	-	5,5,5	0.38	0	5,5,5	0.24	0
5	GOL	B	7	-	5,5,5	0.29	0	5,5,5	0.72	0
5	GOL	A	2	-	5,5,5	0.41	0	5,5,5	0.40	0
7	PGE	A	835	-	3,3,9	0.42	0	2,2,8	0.29	0
5	GOL	A	6	-	5,5,5	0.39	0	5,5,5	0.21	0
7	PGE	C	6	-	4,4,9	0.44	0	3,3,8	0.26	0
8	ACT	A	841	-	1,3,3	1.28	0	0,3,3	0.00	-
5	GOL	C	8	-	5,5,5	0.33	0	5,5,5	0.70	0
5	GOL	A	5	-	5,5,5	0.37	0	5,5,5	0.25	0
8	ACT	A	840	-	1,3,3	0.99	0	0,3,3	0.00	-

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	838	-	-	0/1/1/7	-
4	XJS	A	1	6	-	22/73/90/90	0/2/2/2
5	GOL	A	3	-	-	0/4/4/4	-
5	GOL	A	4	-	-	0/4/4/4	-
7	PGE	A	837	-	-	0/1/1/7	-
5	GOL	C	9	-	-	2/4/4/4	-
5	GOL	B	7	-	-	2/4/4/4	-
5	GOL	A	2	-	-	4/4/4/4	-
7	PGE	A	835	-	-	1/1/1/7	-
5	GOL	A	6	-	-	2/4/4/4	-
7	PGE	C	6	-	-	1/2/2/7	-
5	GOL	C	8	-	-	2/4/4/4	-
5	GOL	A	5	-	-	1/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	XJS	C18-N5	6.98	1.49	1.33
4	A	1	XJS	C19-N6	6.81	1.48	1.33
4	A	1	XJS	C25-N7	6.69	1.48	1.35
4	A	1	XJS	C24-N8	6.27	1.47	1.35
4	A	1	XJS	C11-N4	6.24	1.47	1.35
4	A	1	XJS	C8-N2	6.17	1.47	1.33
4	A	1	XJS	C5-C1	5.37	1.53	1.43
4	A	1	XJS	C4-N3	5.34	1.42	1.33
4	A	1	XJS	C7-C3	4.99	1.54	1.47
4	A	1	XJS	P1-O11	3.59	1.63	1.50
4	A	1	XJS	P2-O9	3.47	1.63	1.50
4	A	1	XJS	C2-N3	2.55	1.43	1.38
4	A	1	XJS	P3-O7	2.48	1.64	1.54
4	A	1	XJS	C20-C18	2.47	1.56	1.51
4	A	1	XJS	P3-O6	2.45	1.64	1.54
4	A	1	XJS	O16-C19	-2.38	1.18	1.23
4	A	1	XJS	C9-C8	2.23	1.55	1.51
4	A	1	XJS	C21-C19	2.20	1.55	1.51
4	A	1	XJS	O18-C25	-2.09	1.18	1.23
4	A	1	XJS	C22-C25	2.09	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	XJS	O15-C18	-2.06	1.19	1.23
4	A	1	XJS	O4-C4	-2.03	1.19	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	XJS	C5-C4-N3	-7.93	118.87	124.40
4	A	1	XJS	C4-N3-C2	6.66	120.77	115.14
4	A	1	XJS	C7-N2-C8	-4.69	116.94	121.60
4	A	1	XJS	C21-C19-N6	2.75	121.06	116.42
4	A	1	XJS	C17-N6-C19	-2.46	118.27	122.84
4	A	1	XJS	C20-C22-C25	2.43	120.76	111.92
4	A	1	XJS	C16-C17-N6	2.40	119.07	112.21
4	A	1	XJS	C16-C13-N4	2.39	119.93	112.44
4	A	1	XJS	C14-C12-N4	2.24	119.48	112.44
4	A	1	XJS	P2-O3-P3	-2.23	125.17	132.83
4	A	1	XJS	O6-P3-O3	2.21	112.03	104.64
4	A	1	XJS	P2-O1-P1	-2.20	125.29	132.83
4	A	1	XJS	O13-C8-N2	-2.12	119.01	123.01
4	A	1	XJS	O12-C3'-C2'	2.12	118.49	110.90
4	A	1	XJS	O15-C18-N5	-2.03	119.19	123.01
4	A	1	XJS	O16-C19-N6	-2.01	119.21	123.01

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	XJS	P2-O3-P3-O6
4	A	1	XJS	C19-C21-C23-C24
5	C	9	GOL	O1-C1-C2-C3
5	A	2	GOL	O1-C1-C2-O2
5	A	2	GOL	O1-C1-C2-C3
5	A	2	GOL	C1-C2-C3-O3
5	A	6	GOL	C1-C2-C3-O3
4	A	1	XJS	C16-C13-N4-C12
4	A	1	XJS	C20-C18-N5-C15
4	A	1	XJS	C33-C31-N7-C25
4	A	1	XJS	C29-C28-N8-C24
4	A	1	XJS	C32-C30-N7-C31
4	A	1	XJS	C27-C26-N8-C24
4	A	1	XJS	O15-C18-N5-C15
4	A	1	XJS	C18-C20-C22-C25

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Mol	Chain	Res	Type	Atoms
4	A	1	XJS	N4-C13-C16-C17
4	A	1	XJS	C29-C28-N8-C26
4	A	1	XJS	C27-C26-N8-C28
4	A	1	XJS	C16-C13-N4-C11
4	A	1	XJS	C33-C31-N7-C30
4	A	1	XJS	C22-C25-N7-C30
5	B	7	GOL	O1-C1-C2-C3
5	A	5	GOL	O1-C1-C2-C3
5	C	9	GOL	O1-C1-C2-O2
4	A	1	XJS	C32-C30-N7-C25
5	B	7	GOL	O1-C1-C2-O2
4	A	1	XJS	C10-C11-N4-C12
7	C	6	PGE	O2-C3-C4-O3
5	A	2	GOL	O2-C2-C3-O3
5	C	8	GOL	C1-C2-C3-O3
7	A	835	PGE	O2-C3-C4-O3
4	A	1	XJS	C13-C16-C17-N6
5	A	6	GOL	O2-C2-C3-O3
4	A	1	XJS	C14-C12-N4-C13
5	C	8	GOL	O2-C2-C3-O3
4	A	1	XJS	P2-O3-P3-O7
4	A	1	XJS	P2-O3-P3-O5

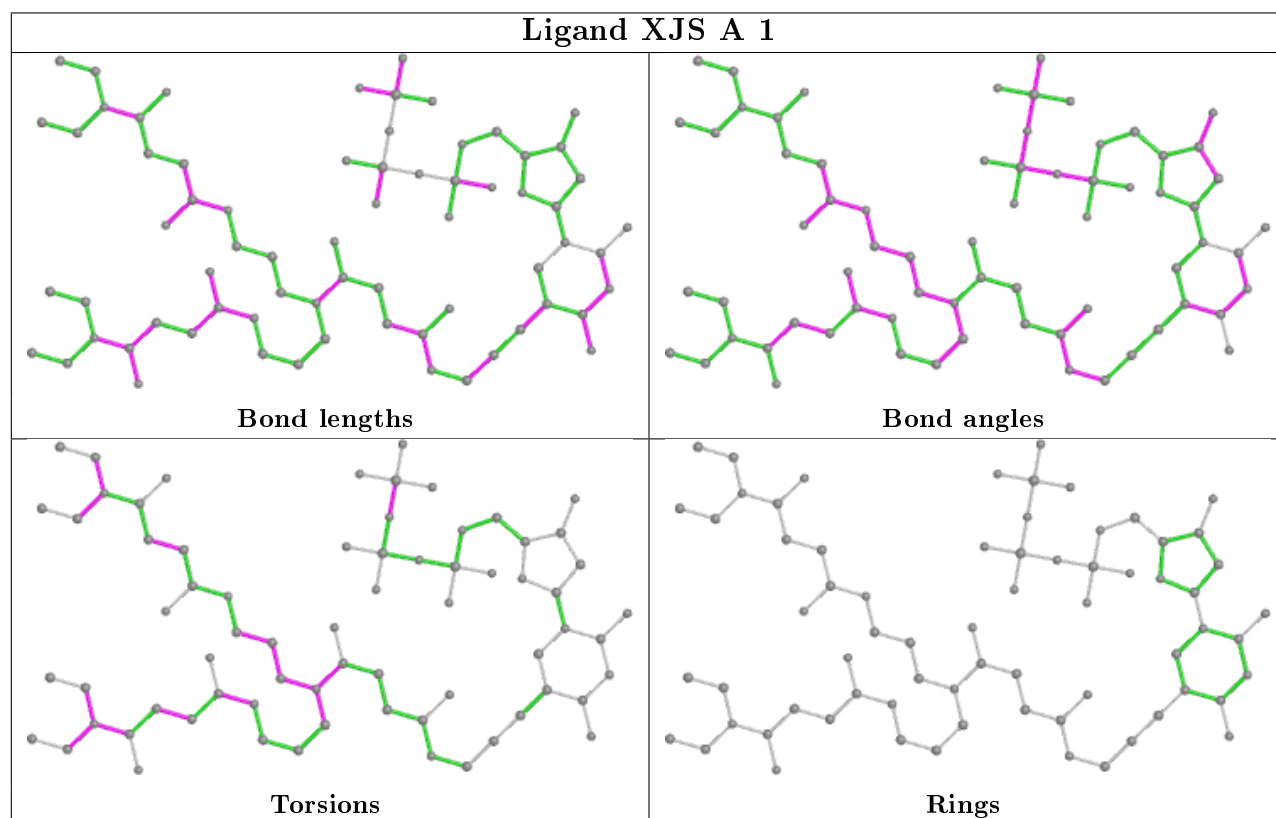
There are no ring outliers.

8 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	XJS	22	0
5	A	3	GOL	1	0
5	B	7	GOL	4	0
5	A	2	GOL	5	0
7	A	835	PGE	1	0
7	C	6	PGE	1	0
5	C	8	GOL	1	0
8	A	840	ACT	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%)	-0.01	24 (4%) 33 36	21, 36, 86, 131	0
2	B	11/12 (91%)	-0.49	0 100 100	25, 28, 57, 58	0
3	C	16/16 (100%)	-0.31	0 100 100	23, 33, 101, 101	0
All	All	566/568 (99%)	-0.03	24 (4%) 36 39	21, 36, 86, 131	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	ALA	6.7
1	A	647	PHE	5.5
1	A	682	LEU	5.5
1	A	644	SER	5.1
1	A	692	PHE	5.0
1	A	683	ALA	4.8
1	A	691	ALA	4.6
1	A	645	TRP	4.4
1	A	648	GLY	3.9
1	A	693	ILE	3.8
1	A	680	GLN	3.5
1	A	688	GLU	3.3
1	A	685	PRO	3.1
1	A	684	ILE	2.8
1	A	698	GLN	2.7
1	A	700	PHE	2.5
1	A	649	VAL	2.4
1	A	697	PHE	2.4
1	A	299	TRP	2.4
1	A	696	TYR	2.3
1	A	699	SER	2.3
1	A	686	TYR	2.3
1	A	695	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	650	PRO	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, 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	0.97	0.10	19,28,37,39	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, 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
5	GOL	A	3	6/6	0.81	0.19	38,69,81,85	0
7	PGE	C	6	5/10	0.81	0.23	44,68,80,80	0
7	PGE	A	835	4/10	0.84	0.29	70,78,93,93	0
5	GOL	B	7	6/6	0.84	0.19	22,48,64,64	0
8	ACT	A	841	4/4	0.88	0.11	52,61,63,64	0
5	GOL	C	8	6/6	0.88	0.16	39,56,68,68	0
7	PGE	A	837	4/10	0.90	0.12	49,67,76,76	0
5	GOL	A	2	6/6	0.91	0.24	42,58,79,79	0
5	GOL	A	6	6/6	0.92	0.20	50,61,71,74	0
5	GOL	C	9	6/6	0.93	0.18	53,64,74,76	0
5	GOL	A	4	6/6	0.93	0.11	31,42,51,51	0
5	GOL	A	5	6/6	0.93	0.21	50,70,86,91	0
8	ACT	A	836	4/4	0.94	0.33	72,74,87,87	0
8	ACT	A	840	4/4	0.96	0.23	27,33,34,35	7
4	XJS	A	1	69/69	0.97	0.15	27,55,111,111	8
7	PGE	A	838	4/10	0.98	0.22	38,49,58,64	0

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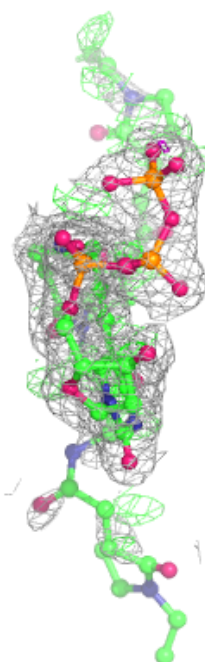
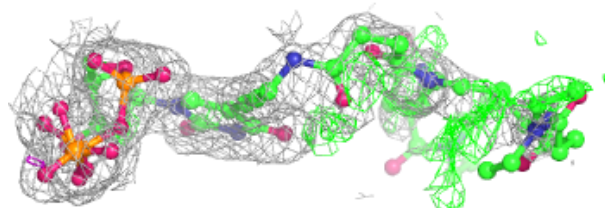
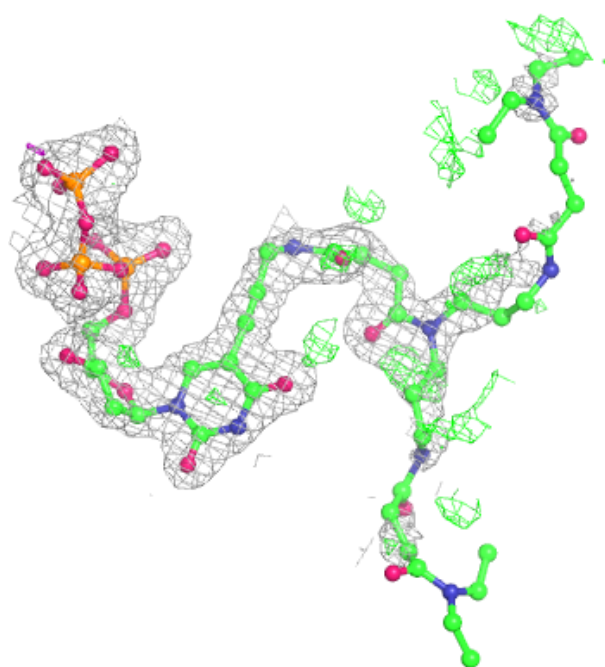
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	A	7	1/1	0.98	0.10	29,29,29,29	0
6	MG	A	8	1/1	0.99	0.09	31,31,31,31	0

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 XJS 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

There are no such residues in this entry.